

# **DATA PROCESSING PROCEDURES FOR UCR EPA ENVIRONMENTAL CHAMBER EXPERIMENTS**

## **Appendix B To Quality Assurance Project Plan**

**DRAFT**

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### **Preface**

This document describes the files and procedures that are to be used for the initial processing of the data obtained from EPA environmental chamber experiments. Responsibilities of personnel with regard to data input, documentation, processing and quality assurance are also described. The functions, formats, and locations of the various computer files involved are documented, and relevant checklists and standard operating procedures with regard to data processing are summarized.

The current document is a draft being circulated to the CE-CERT Atmospheric Processes (AP) group for comments. Once this is finalized, it will be expected that all personnel working on CE-CERT EPA chamber projects will abide by the procedures described herein. Use of these procedures and files may also be required for experiments in other environmental chambers used by the CE-CERT AP group, if so directed by the project manager or Principal Investigator

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## 1 Personnel and Responsibilities

Table 1 gives a summary of the personnel involved in various phases of conducting or processing the environmental chamber experiments. The “designation” column gives the terms that will be used to refer to the various areas of responsibility in the remainder of this document, and the “Description of Relevant Responsibilities” column of the responsibilities that are described in more detail below. Note that some of these areas of responsibility may be shared, but only if one person is identified as being responsible for each of the different areas. In addition, depending on the scope and complexity of the project, one person may assume more than one area of responsibility.

The table also gives the names of individuals that are proposed as being normally responsible for the particular areas, at least for chamber projects that are currently underway. This is subject to change as needs arise. In most cases it is expected that more than two individuals should be able to assume the different areas of responsibility so experiments and data processing can continue if the primary person is unavailable. Likely back-up personnel are indicated on the table.

## 2 Computer Data Files

Table 2 lists the computer files (or types of files) currently involved with data processing for environmental chamber experiments. The current location of these files on the CE-CERT network is also indicated, along with the person primarily responsible for maintaining them. The formats and data contained in the various types of files are described in more detail below.

### 2.1 Run Instruction File

The Run Instruction file is used by the project scientist as the primary means for providing instructions to the people carrying out the experiments about how the run should be conducted. This includes a summary sheet listing the runs to be carried out, and separate Instructions, Injections, and Checklist sheets for each requested experiment on the list. The latter are created by the Project Scientist for each run by using the sheets in the “Run Instructions Template” as the starting point, and filled out as appropriate. When the run is completed, the Primary Run Technician fills the sheets out as appropriate to indicate what was actually accomplished during the experiment, and moves these sheets from the Run Instruction file to the Run Data Files for the runs when the runs are completed successfully. Since these sheets are removed from the Run Instructions File when the run is successfully completed, the file should contain only Instructions, Injections, and Checklist sheets for runs that still need to be conducted.

The “Summary” sheet contains a list of the requested experiment in the order they to be conducted, along with a brief description. (More detailed instructions are given in the “instructions” and “injections” sheets, described below.) It also indicates the temporary run ID assigned to it, which are used to identify the instructions, injections, and checklist sheets for the run. After the run is completed, the Primary Run Technician should enter the run number in the column provided for it once the experiment is conducted, and enter an “ok” or “failed” in the column provided to indicate if it is considered to be a success or will have to be repeated.

The “Instructions” sheets give the instructions from the Project Scientist concerning the experiment to be conducted, except for the reactant injections, which are given in the separate “Injections” sheets. The information in this sheet may vary depending on the type of run, but would

include reactor preparation instructions, desired sampling and span schedules, priority measurements, and special operations and instructions. Provision is made for the Run Technician to enter the run ID and provide comments about what actually was done during the experiment, if they differed from the instructions. Note that information entered by the Primary Run Technician should be in red font, while instructions entered by the project scientist is in black. The preliminary version of the “instructions” sheet is reproduced in Table 3

The “Injections” sheets indicate what compounds are to be injected, how much, when, and into which reactor. It has two sets of columns, one with the “injection instructions” to be filled out by the Project Scientist and one with the “injections as achieved” to be filled out by the experimentalist (generally the Primary Run Technician) after the run is completed. As with the “Instructions” sheet, instructions entered by the Project Scientist should be in black, and results and comments entered by the experimentalist should be in red. The preliminary version of the “injections” sheet is reproduced in Table 4.

The “Checklist” sheets have a checklist of the various operations that should be carried out by the experimentalists (primarily) during the preparation and data processing for the run. The various items should be checked off as they are accomplished. This is discussed further in the “Procedures” section, below. The preliminary version of the checklist is reproduced in Table 5

## **2.2 Run List File**

The run list file contains a log of all experiments conducted. It contains a separate sheet for each chamber, with columns for the run number, date, description, and comments. The Primary Run Technician should add the summary for each experiment as soon as possible after the experiment is completed.

## **2.3 Run Data Files**

The Run Data file is an Excel file that contains data from each experiment, as well as run-specific comments and parameters that are needed for properly processing the data and modeling the experiment. A separate run data file is used for each experiment. These files contain a number of different sheets with different types of information, as indicated below. Except as indicated otherwise below, the Primary Run Technician is responsible for correctly entering and processing data in this file.

A complete description of all the data in the run data files is given in Table 6. Responsibilities for entering and maintaining the data in this file and procedures for processing these data are discussed later in this document. Given below is a brief description of the various types of sheets and the major information that need to be entered and maintained, and other considerations involved.

The “Instructions”, “Injections” and “Checklist” sheets are the corresponding sheets taken from the Run Instructions File that are moved to the Run Data File when the latter is created. These were described above.

The “Log” sheet gives the major run parameters, general documentation, and user input flags associated with the experiment. At the very minimum, the data start and end time must be given before any data can be loaded and processed. Times for major run events such as turning the lights on and off and completion of injection of reactants should also be entered where appropriate. This sheet is also used to indicate states for the data if they are different than computed from the flags output by the data acquisition system, and to flag nonstandard data for particular instruments. It is essential that any non-

standard states be flagged appropriately for the data to be processed correctly. Procedures for doing this are discussed separately in the “Data Processing Procedures” section.

The “Data File Control” sheet is used to indicate which data files contain the data acquisition and other continuous monitoring data for the run, and give parameters indicating their format. If the only files input are those that the data acquisition system or usually connected instruments that are in standard locations and whose names are based on the date, the template should already have the appropriate names computed based on the run start and end times. In these cases, it may not be necessary to modify or enter any new data on this sheet. However, if files with non-standard names, locations or formats are used, the appropriate information may need to be input manually.

The “Data Channel Control” sheet is used to provide the necessary information to load and process the data for all the data channels interfaced to the data acquisition system (DAS), as well as any other channels whose data are obtained from files given in the “Data File Control” sheet. Note that the ordering of the channels should be preserved since it affects how the data are plotted when the data plotting and control file is used for data processing, with new channels added at the end. It may not be necessary to manually enter information on this sheet if the connected instruments and species being monitored are appropriately represented in the template, but this should be checked for each experiment. Once the data are loaded and initially processed and assigned to the appropriate state (with entries being made to the “Log” sheet as needed to appropriately assign states and reject bad data as needed), then the macros accessed on this sheet can be used to compute zero and span corrections for channels where this is appropriate. However, appropriate factor and zero offset corrections will need to be manually entered for any channel where corrections are needed where they cannot be calculated from the span and zero data for the run. This is discussed further in the “Procedures” section, below.

The “Cal Sources” sheet is used to give the span concentration information for all span gases that are sampled during the experiment, if it is desired to use these to compute span correction factors for any channels. Although the template has default values, these should always be checked for appropriateness for each experiment, and even if the defaults do not need to be changed, the “date last checked” and the “other cal source documentation” columns should be filled in appropriately. This is necessary to assure that the experimentalists have checked these values for correctness, and the default values are not being used because no one has bothered to check them.

The “GC Data” sheet is used to enter the GC data taken during the experiments. At the present time all these data need to be entered manually, but eventually macros will be written to automatically read GC data from HPCHEM files, provided they are named and located as indicated in Table 2.

The “Sample Inlet Control” sheet is used to provide information on how the valve states and other flag channels read in with the data files are used to determine the sampling states of the associated data channels. Usually this is not modified unless the sampling state configuration is modified. The data processing manager should be notified if the sampling configuration is modified in such a way that it cannot be described by the parameters and format given in the current template.

The “Model Input” sheet is used to prepare the input files needed to conduct model simulations of the data from this experiment. Preparing the data on this sheet is the responsibility of the run modeler, and unless instructed otherwise the run technicians and instrument operators need not be concerned with this sheet.

The “Loaded Data” sheet is used by the data input macros to store the raw data and flag values that are read in from the files in the “Data File Control” sheet for the channels listed in the “Data Channel Control” sheet. It is not used for GC data. Normally the run technicians and operators do not need to work

with this sheet, which is output and read only by the data loading and processing macros. However, they may wish to view this sheet to determine if data were loaded as expected. Data should not be manually edited on this sheet; rejected data should be indicated by appropriate entries in the “Log” sheet as indicated on Table 6.

A number of Processed Data Sheets are produced by the data processing procedures, with a separate sheet being created for each sampling state used. The data on these sheets are over-written every time the data are re-processed (as would occur whenever any correction factors or sampling state flags are changed). Therefore, they should never be manually edited. The data on these sheets are copied to the data plotting spreadsheet file for plotting and data on the sheet(s) for the reactor state(s) are used for model evaluation.

Note that several color codes are used to indicate the types of data in the various sheets, as indicated by comments in the “Log” sheet. These are as follows:

- Black is used for data, comments, or headers, and also for defaults for data or parameters that should be changed only infrequently.
- Red is used for data, parameters, or other information that should be modified or at least checked when the data are entered for each experiment.
- Blue is used for calculated data. Cells with blue characters should never be modified or deleted, though if cells are added it may sometimes be appropriate to copy them there.
- Purple is used for data created by macros. Cells with such data will be over-written when the appropriate macro is run.

These same color codes (or at least blue for calculated cells) are used in most of the other files used for chamber data processing. These are useful for determining which cells can or should be modified or updated for individual runs or which should not be modified either because they are constant or are calculated by a spreadsheet formula or macro. Note that cells with spreadsheet calculations may need to be copied from appropriate locations if columns or rows are added to make room for additional data or entries.

Exceptions to this color coding convention are the sheets copied from the Run Instructions File. In these cases, as discussed above, the convention is to use black for instructions entered by the Project Scientist prior to the experiment and red for data and comments entered (usually by the experimentalists) based on what was actually occurred during the experiment as conducted.

## **2.4 Current Data File**

The file “EPAdata.xls” is a special run data file that can be used for viewing plots of data collected using the data acquisition system, without the data necessarily being associated with any particular experiment. Although not strictly speaking used for data processing, it is a convenient means to assess data as they are being collected, or before any run files are created. The user selects the days for which the data are to be viewed (the default being “today”), and then runs the macros to load, process, and plot the data. For it to operate, all the raw data files for the selected time period must be on line with their default names and in their default locations. The Data Processing Manager is responsible for this file being configured properly to represent the current DAS configuration.

## 2.5 Run Data Control and Plotting File

This Excel file contains the macros used when loading and processing the run data in the run data file, and it is also used for plotting the data in the runs. The operations of the macros are described in Table 8 and also in the discussion of the data processing procedures, given below.

The “Plots” sheet is the only sheet that the user would normally need to access when viewing or processing data for a run. It contains plots of the major measured channels in the zero, reactor, and enclosure for most channels, and span state data for species of relevance for those states. Macro buttons on the side can be used to change the runs whose data are being viewed, to view the currently linked run data file, to create new runs, or to go to columns for selected groups of plots.

The “Control” sheet contains data and parameters that the macros use to determine which run file is being viewed or processed, and contains other parameters that are used in creating the plots for the experiments. The data in this sheet would not normally be modified except under operation of the macros, unless the data to be plotted are to be changed. In that case, the modifications are usually made by the Data Processing Manager or the person responsible for maintaining this file. Note that the data in this sheet affects only how the data are displayed in the “Plots” sheet of this file, and has no effect on how the run data are processed and stored in the run data file.

The rest of the sheets contain the data for the various states that are plotted, one sheet for each state. The states whose data are plotted are listed in the “States” section of the “Control” sheet, and there must be one sheet for each such state. When the data from a run is to be plotted, the macros linking the data to this file copy the data for these states from the processed data sheets in the run file to these sheets.

## 2.6 Control Parameter File

This file, named “ChamWork.xls”, is used to provide the data processing procedures in the run data control and plotting file with parameters that may vary from computer to computer, and is also used to cause the data control and plotting procedures to be loaded. It must be installed in the C:\Chadpro directory on any computer where the data processing using the Run Data Control and Run Data files are to be used. Loading this file will cause the Run Data Control and Plotting file to automatically be loaded, provided its location is specified correctly in this file. Most of the macros used for data processing require this file to be loaded, and if it is not loaded when the macros are run, they will look for it in the C:\chadpro directory and abort if it is not found.

The control parameter file currently has a single sheet (named “Parm”) that contains file names and network locations for the files and sources of data that the data processing program uses or may use. It should be normally edited only by the data processing manager.

## 2.7 Valve State Control File

The Valves.xls file contains information defining what is being sampled for each set of valve configurations. It also contains definitions of named sample states and sampling schedules, and contains macros to output sampling schedules in a format that can be used by the valve control program for the sampling system. Strictly speaking this file is used for controlling sampling during an experiment and is not used for data processing. However, the valve state definition sheet in this file **MUST** be consistent with the valve state definition information given in the “Sample Inlet Control” sheet in the Run Data file. Normally the Primary Instrumentation Technician is responsible for maintaining this file.

The “Valve State Definition” sheet indicates which valves are activated for sample to be input from the various sampling states. Although the state numbers and descriptions do not have to be exactly the same as used in the run data files, at least the numbers should be consistent to avoid errors and to make it easier to assure that the valve states are being appropriately represented in the “Sample Inlet Control” sheet in the Run Data file. The “Abbrev” column gives the abbreviations used for the states in when defining the sampling cycles in the “Cycle Definitions” sheet.

The “Cycle Definitions” sheet can be used to create named sampling schedules that can be used when running the valve control program for experiments. The files are given names given in the “Name” row for the various cycles, with the extension “.vfv”, and are output in the path indicated on the “Output Path” line in the “Valve State Definition” sheet. The format of the data in the cycle definitions sheet and the operation of the macros to define the cycles is described in the “Documentation” sheet in this file, and is thus not discussed further here.

The “Documentation” sheet describes the format of the “Cycle Definitions” data and how to operate the procedures to make cycle definition files for use by the valve state program. It should also be used to add other documentation related to the valve setup as appropriate.

The “Sampling Setups” sheet describes the various sample configurations corresponding to the “Sampling Setup” code given in the “Sample Inlet Control” section of the run data sheets. It indicates when the various setups were installed and also the location of the log book page or document that describes the setup in more detail..

The “Work” sheet is used by the macro when creating cycle definition files, and should not be directly modified by the user. It contains the last sample state definition file that is produced.

## **2.8 Instrumentation Information File**

The InstInfo.XLS file contains descriptions of all instruments currently employed by the CE-CERT AP group, their model and serial number, and the designation used for each in the run data and other data processing files. It also contains information on which species the instruments monitor and how they are interfaced to the data acquisition system. The Primary Instrumentation Technician is responsible for maintaining this file.

This file does not normally have to be modified unless new instruments are acquired or their connections to the data acquisition system are changed, and does not normally need to be accessed when processing data for an experiment. However, steps should be taken to assure that the instruments used during the experiments are properly identified using the instrument ID codes that are associated with each instrument in this file.

The “Data Logger Inputs Outputs” sheet contains information about the data logger channels in a format that is useful to the maintainer of the data acquisition system. The information in this sheet should be consistent with the information in the “DAS Connections” sheet, described below.

The “DAS Connections” sheet contains information about the data logger channels in a format that is useful for those responsible for data processing. One row is given for each data channel that is or may be used in chamber experiments. The following information is given for each such channel:

- “DAS Chan ID” ... The identification used for this instrument/species combination in the run data sheets, as given in the “Channel Name” column in the “Data Channel Control” sheet of the run data files.



- “On Line” ... “1” indicates that the instrument is currently connected to the data acquisition system, blank indicates it is not. Alternately, the Primary Instrumentation Technician may prefer to give the channel number used, if applicable.
- “DAS Header Code” ... indicates the code used in the header of the primary DAS output file to indicate this channel. The Primary Instrumentation Technician should assure that this matches the header that is actually used. Note that this is referenced in the “Data Source Label” column in the “Data Channel Control” file for channels that are read from the primary DAS output file.
- “Species” ... the Chadpro name of the species or parameter whose data are being reported in this channel.
- “Instrument” ... The Instrument ID code for the instrument being used. It must match the ID codes given in the “DAS Instruments” sheet.
- “Zero Meth” ... A code indicating how the zero corrections should be applied, ranging from “0” for no such correction is appropriate to “3” for corrections should be made on a run-to-run basis. This should be obtained from the SOP for the instrument. See discussion of data processing procedures, below.
- “Default Zero” ... The zero offset correction that should be used if this has a “Zero Meth” code of 0 or 1, or the default value that should be used if no data are available
- “Span Meth” ... A code indicating how the span corrections should be applied, ranging from “0” for no such correction is appropriate to “3” for corrections should be made on a run-to-run basis. This should be obtained from the SOP for the instrument. See discussion of data processing procedures, below.
- “Default Span” ... The span correction factor that should be used if this has a “Span Meth” code of 0 or 1, or the default value that should be used if no data are available
- “Instrument Description” ... This is the description associated with the ID given in the “instrument” column as found in the “DAS Instruments” sheet. If it contains “N/A”, then the ID isn’t found on the sheet, and either the correct ID should be used for the instrument, or the instrument is new and needs to be added to the “DAS Instruments” sheet.

The “DAS Instruments” sheet contains the ID designation, description, manufacturer, model, serial number, outputs, and other information for all of the instruments available at CE-CERT that can or may be interfaced with the data acquisition system. This should include “loaner” or collaborator’s instruments that are used on a temporary basis if the data are used in any experiments or study. The first column contains the 8-character (maximum) that is assigned to that instrument, which must be unique and also be a legal DOS file name (i.e., it should contain no embedded blanks and consist of only alphanumeric characters, or “\_” or “-“ characters.) The other columns are reasonably self-explanatory and all should be filled in for each instrument where applicable.

The “GC Instruments” sheet contains the ID designation, description, and other relevant information for GC instruments currently in use. The information contained in this sheet may eventually be enhanced or modified as the GC data processing procedures are further developed.

The “Spectral Instruments” sheet contains the ID designation, description, and other relevant information for the instruments in use that output array data of various types. This currently includes only spectral measurement instruments, but it will eventually also include instruments that output particle number and size distribution data as they become on line. The information contained in this sheet may eventually be enhanced or modified as the array data processing procedures are further developed.

The “Old Chadpro List” sheet contains the old Chadpro ID numbers and descriptions used for instruments as of 1995. This is for archiving purposes and should not be modified.

## **2.9 Calibration Information Files**

The quality assurance project plan and standard operating procedures being developed for the EPA chamber project will call for using Excel or database files to tabulate calibration history and other relevant information for the various instruments where this is relevant. The formats and data contained in these files will depend on the instrument. This has not yet been implemented.

## **2.10 Raw Data Files**

As indicated on Table 2, the data acquisition program and some of the instruments output various files with the raw measurement data, and in most cases their contents can be read into the run data files using the data processing programs. The locations and formatting information must appropriately specified in the “Data File Control” sheet in the run data file as indicated in the discussion of this sheet in Table 6. The current CE-CERT network locations used for these files are given in Table 2. The formatting parameters that should be used when reading data from these files as currently configured is given in Table 7. The run template should have the appropriate parameters for the types of files that are normally read, which presently includes the DAS primary data files and the valve state files.

At present the data processing procedures associated with the EPA chamber do not read the GC data files produced by the HPCHEM program, but previous Chadpro utility programs can read these data, based on file locations and naming conventions as indicated on Table 2. Eventually these old Chadpro utilities will be adapted for use with the new data processing procedures and files, so these locations and naming conventions should be retained.

Further discussion of the format of these raw data files is beyond the scope of this document.

## **3 Use of the Data Processing Files and Macros**

As indicated on the checklist template on Table 5, most of the data processing procedures consist of filling in, processing, and checking information in the Run Data File for the experiment. The Run Data Control and Plotting file contains the spreadsheet macros and the plotting capabilities needed to carry out these operations in the most efficient manner available. This is “linked” to a selected Run Data File (or the “Current Data file”) that actually contains the data and parameters to be entered, manipulated, and viewed. The linked run data file must be chosen and opened before most of the procedures can be used. Macros are included that can be used for this purpose, as discussed below.

### **3.1 Installation**

The data processing and procedures can be run on any Windows computer on the CE-CERT network whose user has read and write access to AP group shared files that has a legal copy of Microsoft Excel (97 or 2000) installed. (It has not been tested with Excel 2002 or higher.) The computer should have sufficient memory to run large Excel spreadsheets reliably and be sufficiently rapid that the data processing macros do not take excessive time. The data processing procedures can be installed and run on more than one computer at the same time, though obviously the same Run Data file cannot be edited at the same time. However, different people can simultaneously edit run files from different experiments, and different people can simultaneously use the Current Data File to view plots of data.

It is also necessary that Excel macros not be disabled on the computer being used. Check the “Security” settings in the Excel “Tools” menu and make sure the security in the “security” tab is not set at

“high”. If it doesn’t say that a virus scanner is installed at the bottom of that menu, then have Systems install Norton Anti-Virus or an equivalent virus scanner that is capable of checking macros. In the meantime, set security to “medium” so the macros will run, though you will be warned every time you load the files. Once a virus scanner is installed, you can set it to “low” and not get the warning every time.

Installation consists simply of creating a “C:\Chadpro” directory on the local computer to be used, copying a version of “ChamWork.xls” to it, and entering in its “parms” sheet the appropriate network paths for the files and data locations that will be used. Most of the network paths will be the same for all computers on the CE-CERT network, and need not be edited for individual computers. These paths are as indicated on Table 2. The main exceptions are as follows:

- The “LocalID” parameter should give the name of the local computer on the CE-CERT network. (This is not currently used by the macros, but should be provided for future use.)
- The “TmpDir” parameter should give a valid path on the local computer that can be used for temporary files, since the macros will fail if that path does not exist. Normally this would be “C:\temp”, which is what Windows uses for temporary files on most computers, but some users may prefer to use different temporary directories. (This is used mainly to copy raw data files before they are opened, to avoid problems with opening data files that may still be written to by DAS programs. Because of a bug in Excel, macros cannot open non-worksheet files in “read-only” mode.)
- The “AllowChadMacroEdits” parameter should be “no” on all computers except for the one used by the Data Processing Manager. Otherwise, there will be conflicts when more than one person attempts to use the procedures, users who are not careful could damage the data control and plotting file, and the Data Processing Manager will have a more difficult time maintaining the programs and files.

The installer should assure that the intended user has read-write access to all the network locations given in the control parameter file. Once this is complete, a shortcut to this file should be created on the user’s desktop or some other location convenient to the user, since this is used to start the data processing or viewing session.

### **3.2 Starting Data Processing Session and Selection of Linked Data Files and Plot Data**

Once the Control Parameter File is properly installed and configured on an appropriate computer, the data entry or processing session can be initiated by clicking on its icon or by selecting “C:\Chadpro\ChamWork.xls” using the Excel “open” command to cause it to be loaded into Excel. If there is a warning about macros the user should select to enable macros or the procedures cannot be used. The macros in the Control Parameter File will then load the Run Data and Control Plotting file (“EpaPlot.xls”), and this process may take some time because the many plots make it is a large file. Note that this step will fail if the network is down or if the user does not have rights to access AP shared files.

Once the EpaPlot.xls file is loaded, the user will see a series of plots in the main frame, and smaller frames to the left and on the top with a series of control “buttons” for running various macros. Some of these can be used for opening or changing the linked data file, and others can be used to change the currently selected file or series of plots. The controls that involve selecting and changing the linked data files are as follows:

- The “Change Run” control is used to select an existing experiment’s run data file for viewing or editing. The user will be prompted to give an experiment name, with the default value being the currently selected run data file (if any). The run file will be loaded and the plots will be updated to reflect the processed data in that run, if any. Although the file (if it exists) will be loaded, the active workbook will continue to be EpaPlot.xls. The “go to file” control can be used to switch to the selected run file as the active workbook, if desired.
- The “New Run” control is used to create the run data file for a new chamber run. The user is prompted to give the run ID. Note that for EPA runs the ID should be of the form EPAnnn, where “nnn” is the three-digit run number, starting at “001”. The next available run number should be used. The run file will be created from a blank template, the run ID will be added to the place for it in the Log sheet, the file will be saved, and the active worksheet will be changed to the new run file.
- The “Current Data” control is used to load the “Current Data” file (EPAdata.xls) so you can view data as it is currently being collected, or other data in the raw data files that may not necessarily be loaded into a run file. This causes the current data file to be loaded (if it is not loaded already) and the active window to switch to that file. However, the data from that file is not automatically loaded into the plots because usually it has to be loaded and processed first. The operation of the “Current Data” file is discussed separately below.
- The “Go to File” control is used to conveniently make the linked file the active window, so edits, etc., can be made. It’s effect is the same as going to the Excel “Window” menu and selecting the linked file.
- The “Reload” control is used to re-load the processed data from the linked run data file into the sheets used to create the plot. If the linked file is the “Current Data” file, it also re-loads all the raw data into the current data file before loading them into the plot file.
- The “View” controls are used to shift the plot frame to the plots for the selected channel, which is designated in blue font above the control. These are handy to view a selected plot on the page that is out of range on the screen. They do not affect the data in the linked data file or change the data being plotted.

**IMPORTANT:** If you use the “Change Run” macro to open a run file to edit that is already being open for edits by someone else, the file will be opened successfully, but it will be opened read-only. The “Change Run” macro may detect this and ask you if you wish to continue, but this hasn’t been checked to determine if checks in all circumstances. You can tell if the file is opened read-only by looking at the title bar on the window, since if it is opened read only it will have a “[Read-Only]” after the file name. You will not be able to save edits when it is opened read-only, so if you intend to make edits, close the file and wait until whoever has it opened is finished before working with it.

### **3.3 Procedures for Loading and Processing Run File Data**

The data control and plotting file has a number of macros that can be used for loading and processing data in run files that will be useful when carrying out the data processing for the completed chamber experiments. Although the control and plotting file must be loaded in order for these macros to be used, they are all used when the run data file is the active Excel window. If the plot file is the active window, use the “Change Run” or “New Run” to select the run file to work on (if it has not already been selected), then use the “Go to File” control to make the run file the active window. The “Go to plots” control on most of the run file sheets can be used to return to the plotting file to view the plots when desired. Normally the data control and plotting file will be loaded whenever working with run data files, but if it is not it will be loaded automatically whenever an attempt is made to run one of these macros using a control in the run data file.

Table 8 describes all the controls and macros currently available for loading or processing data in the run data file. Note that not all of these controls are available on all of the sheets in the run data file, though generally the ones that will be used when working with particular sheets are available on that sheet. For example, the “Data Channel Control” and “Log” sheets have “buttons” for all the data loading and processing macros, the “GC data sheet” has the button for the macro to process only GC data, and the “Model Input” sheet has access to the macros to output model input files.

The ways that these macros would be used when processing data for individual experiments are described in more detail in the “Data Processing Procedures” section, below.

### **3.4 Procedures for Viewing Current Data**

As indicated above, the “Current Data” file is a special run data file that can be used to view the current data or data from previous days that may not necessarily be in a run file. It contains most of the same sheets and data as the template file used to create current run files, with some modifications made to the “Log” and “Data File Control” sheets to make it more convenient for processing current data. The ways that it is normally used is summarized in this section.

When the file is loaded, the “Data File Control” sheet should normally be what is selected. At the top there is a cell labeled “Start Date” that is used to select the starting date for the day to be viewed. If it is blank, the current day (i.e., today) is used. Underneath that is a cell named “Number of Days”. Enter 1 for viewing data for a single day, or 2-5 for viewing data for up to five days starting at the start date. Negative numbers can be used for viewing data for days before the start date given, which is useful when the start date is today. I.e., if the start date is blank and the “number of days” is -1, the data for today and yesterday are displayed. The start and ending times in the “Log” file are computed based on these dates, with the times going from midnight to midnight.

The “Initialize”, “Load Data” and “Process Data” macros must be run in that order to load the data and process it and copy the processed data to the plot file where plots of it can be viewed. The “View Plots” macro can be run to make the plot file the active Excel workbook so the plots can be seen. A “Load and process data, then goto plots” macro is available on the “Data File Control” sheet of the current data file to conveniently do this all at once. If the plots are being viewed, the “reload” macro can be used to update the current data for the current time without having to go back to the current data file.

Since the data in the current data file changes every time it is used, it is not usually saved except after being modified by the Data Processing Manager. Therefore, if the “Current Data” macro on the plot sheet is used to load the file, it is opened read-only unless the “AllowChadMacroEdits” parameter in the ChamWork.xls file is set to “yes”, which should be the case only on the computer being used by the Data Processing Manager.

## 4 Data Processing Procedures

Given in this section are the procedures that should be followed when processing data for chamber experiments, and instructions for operating the programs and macros that were incorporated in the run data control file for this purpose. Most of the data processing procedures that should be followed are indicated in the “Checklist” sheet in the Run Instructions File template, which is reproduced in Table 5. This checklist template is used to create the checklist for each experiment, with additional data processing items being added when necessary for runs that involve additional or special data processing procedures. These items should be checked off in the run’s checklist sheet when they are completed.

Given below is a summary of the major aspects of the data processing procedures, along with a discussion of how to operate the various spreadsheet programs and macros that are available to aid the data processing effort. However, the checklist for the particular experiment should be consulted for a complete list of the data processing operations that are required.

### 4.1 Run Instruction Procedures

Prior to the experiment, the project scientist will provide instructions for carrying out the experiments, giving the desired injections, irradiation times, special procedures and operations, and type of sampling schedule to employ. This is done by creating new run instructions and injections sheets using the run instructions template (\\ozone\apldata\chambers\templates\NewInstr.xlt), adding the filled-out sheets to the run instruction file (\\ozone\apldata\chambers\RunInstr.xls), and indicating on the summary sheet on that file the desired ordering for the experiments to be conducted. The data processing procedures checklist sheet is created from the template and added to the run instructions file during this process. At this point, the Project Scientist may add additional items to the checklist if needed for this particular experiment.

The Primary Run Technician will then examine the summary sheet in the Run Instructions File to determine which experiments need to be carried out and in what order, and then examine the Instructions and Injections sheets for the individual requested experiments for details concerning the requested runs. He or she will be responsible for contacting the Project Scientist if there are missing instructions, ambiguities or needed clarifications, if there is some reason why it may be difficult to follow the instructions as stated, if he or she may prefer a different run ordering than requested, or if he or she feels that better results would be obtained if different procedures were followed. If the instructions are revised, the revised instructions will be entered in the run instruction sheet. Generally the Project Scientist should enter the revisions in run instructions to the sheet. If any one else makes revisions they should be with the approval of the project scientist, the original instructions should not be deleted, and the revised information indicating what will be done instead will be entered using red font, with a notation indicating who made the entry.

The Primary Run Technician must approve the Run Instructions and Injections sheets before the experiment is conducted, and if the instructions had to be modified based on discussions with the Project Scientist he or she should assure that the Instructions and/or Injections sheets are revised accordingly. The Primary Run Technician should then check off the “Run Instructions Reviewed and Accepted by Run Technician” item on the checklist.

## **4.2 Procedures During Experiments**

The Primary Run Technician will be responsible for assuring that the experiment is conducted according to the run instructions and that the standard operating procedures for the EPA chamber runs. If the run instructions do not indicate all aspects of the procedures to be followed, then the standard operating procedures should be followed. If there is an inconsistency between the run instructions and the general SOP, then the run instructions take priority.

All operations should be recorded in the log book at the time they are carried out and any problems encountered should be noted as soon after they are noticed as possible. Operations that affect the sampling state or problems encountered with instruments that affects their data or what they are sampling are particularly important to note, along with the time that the data will first be affected.

Before data acquisition for the experiment begins, the Primary Run Technician should assure that sampling schedule is consistent with the agreed-upon run instructions. He or she should also assure that the clock on the data acquisition computer agrees within 30 seconds with clocks that are linked to NIST time. If they disagree then the data acquisition and valve control programs should be stopped, the clock corrected, then the programs should be re-started, and the need for the time correction entered in the Log book.

## **4.3 Data Processing After Experiments**

### **4.3.1 General Experiment Documentation and Logging**

Once the experiment is complete, the Primary Run Technician should log the experiment and enter the description and comments as appropriate in the “Run List” file, and give the completed run number in the appropriate column in the “Summary” section of the Run Instructions File. If the instructions on the Instructions sheet could not be followed exactly, the modifications or problems should be indicated on the spaces provided in the “Instructions” sheet, or these spaces should contain the notation that the instructions were followed (a simple “ok” is sufficient in this case).

### **4.3.2 Creating Run File**

The most convenient way to create the run file is to use the “New Run” that is accessible from the plot sheet that is active when the data processing files are loaded. Enter the appropriate run designation at the prompt. This will create the run file using appropriate template and save it in the appropriate network location, and also assure that the correct run ID is given on the top of the Log sheet. The Run file will then be in the active Excel window and can be edited.

After the run file is created, the “Instructions”, “Injections”, and “Checklist” sheets for this run should be moved or copied from the Run Instruction file to the Run Data file. Note that sometimes Excel crashes when sheets are moved from one file to another, so work should be saved before this is done. These sheets should be moved (i.e., deleted from the Run Instructions File) if the run is considered to be successful and is does not have to be repeated, or is copied if the run has to be re-done. (Note that Excel has a bug that does not allow full sheets to be copied properly from one workbook to another by dragging and dropping the sheet tabs, as one would do when moving sheets. To copy the sheets, create a blank sheet on the destination file, then copy all the contents of the sheet from one to the other using the copy and paste commands.) In the latter case, the operator-entered data about the specific experiment should be deleted from the sheets remaining on the Run Instructions File, though obviously they should be retained in the sheets copied to the run file. Be sure to save the Run Instructions file after these sheets have been moved from them, but not until the run data file with the moved or copied sheets has been saved first.

At this point the sample state codes listed in the “Log” file should be checked for appropriateness and completeness. If the number of sides or reactors used in the run for which useable data were obtained is different than indicated on the template, then the appropriate corrections should be made to the “Side ID” and (if necessary) “Chadpro Output File” columns.

### 4.3.3 Enter Major Run Times and Documentation

Before any data can be loaded the data start and end times should be entered into the “Log” sheet. The former should be some time immediately before data of any potential relevance to the experiment is collected, and the latter should be immediately afterwards. Note that is better to have too broad a range of time and have irrelevant data loaded in the file than to have too narrow a range and exclude data that may eventually be of potential relevance for characterizing the experiment or performance of the instruments. The other major run times should also be entered, as indicated on the Checklist (on Table 5).

The run description and purpose for the run should be entered on the “Log” sheet where indicated; usually these can just be copied from the “Instructions” sheet. The “General Comments” section should include comments about problems or special operations for the run. It is not necessary to duplicate information that is in the “Instructions” sheet, but reference should be made indicating that special operations or problems are involved, and additional information is available on that sheet.

The Event Log section should be used to give a chronology of the major operations made during the experiment, giving the time for each as exactly as possible. Since these should have been written in the log book at the time the experiment is run, this would be copied from the log book. If the operation changes the sampling state of all the instruments on the main sample line and this is not accounted for in the flags output by the DAS system that normally indicate the sampling state, then the state number (or an “x” to indicate unusable data) should be indicated in the “State” column in the “Event Log” section. Otherwise, this column should be left blank. If an entry is made to the “State” column to indicate a non-standard state or rejected data, then an “A” should be entered in a subsequent line for the time when the regular sampling flags can again be used. Otherwise the last state code (or “x”) is used for all times after the last state code entry. All entries in the “Event Log” must be in ascending chronological order or the “Process Data” or “Update Flags” procedures will abort with an error message. Having the exact same time in adjacent lines is acceptable, though if state codes are entered only the last non-blank one will be used.

Note that state codes given applicable only to those DAS channels identified in the “Data Channel Control” as having a sample line (“Samp line”) code of 1, which is used for the main sample line that most of the instruments are attached to. Other sample line codes may be assigned to channels either because they are not connected to the main sample line or because their sampling states may be reflected by different combinations of flag values than the other instruments on the main sample line. Also, there may be cases where the state code for only one channel needs to be changed, as would be the case if an instrument goes offline or is manually attached to a different sample source. In those cases, the state information is entered in the “Offline or non-standard states for selected Channels” section of the “Log” sheet. The channel name is entered in the “Channel” column to enter states for a single channel, or “line *n*”, where “*n*” is the line number, is entered in that column to change states for all instruments on some sample line other than 1 or 0.

Note that channels assigned “line 0” cannot have their states changed from that specified for it on the “Sample Inlet Control” sheet. This line code is generally used for measurements, such as light intensity or some temperatures, where sampling states are not applicable. If it is necessary to change the state for such a channel, give it a new line number and add an appropriate entry for it to assign the default state to it using the “always” type, as described on Table 6.



Often after the data are loaded the plots will indicate that there are cases where the state assignments may need to be modified, and some data may need to be excluded. The process for doing this is discussed separately below.

#### **4.3.4 Load DAS Data**

Before loading the DAS data it is necessary to assure that the appropriate data start and data end times are entered on the “Log” sheet and the correct information is given in the “Sample Inlet Control”, “Data File Control” and “Data Channel Control” sheets as indicated in the checklist in Table 5. (See Table 6 for details concerning the parameters involved.). Once this is done, then the “Initialize” and “Load Data” macros can be run, as described on Table 8. The “Loaded Data” sheet can be checked to see if all the channels that should be loaded in fact were.

#### **4.3.5 Make Sample State and Flag Corrections Needed**

Once the data are loaded, the “Process Data” macro can be run to obtain an indication of what the data assigned to the various sampling states look like. At least some (though not necessarily all) of the cases where there are problems with the data or state assignments should be evident from the plots. The “View Plots” macro can be used to move from the run data file to the plot file to view the plots of the data, and the “goto file” can be used to go back from viewing the plots to editing the run data file.

At a minimum, clearly bad or inappropriate data should be removed or reassigned for the priority data channels for the zero and applicable reactor and span states. Inappropriate data should be removed from zero and applicable span states even for channels where automatic zero or span corrections are not made, since the averages for these states provide a quality check on the appropriateness of the zero and span values that are used.

The procedure for removing the inappropriate data involves first checking the plots to see the times the inappropriate data occur. (If the series with the data in the plot is selected the time will show when the cursor is moved over a point – at least in Excel 2000). Appropriate state or “do not use” (“x”) entries should be made in the “Event Log” or the “non-standard states” section of the “Log” sheet for the applicable periods, then the “Update Flags”, “Process Data”, and “View Plots” procedures can be run to re-process the data and view the resulting plots. This will be an iterative process that should be continued until clean plots are obtained for the channels and states of interest.

Note that the data values in the “Loaded Data” sheet should NEVER be manually edited or deleted. In addition to being an inappropriate data management and documentation practice, such edits would over-written if the data ever have to be re-loaded. Likewise, data in the various processed data sheets for the various states should also never be manually edited, since they would be over-written every time the data are re-processed, which is done any time factor, zero, flag, or other edits are made.

Care should be taken not to reject potentially valid data from reactor states just based on what it looks like, only data where there is a reason to expect the state may be inappropriately assigned or that are clearly invalid should be re-assigned or flagged as unusable. If there is a not known reason to reject or reassign questionable data in reactor states, then they should be retained.

On the other hand, it should be much more obvious when data in zero or span states are questionable, since if the instrument is operating properly at least reasonably constant readings should be obtained. In those cases it is better to err on the side of rejecting questionable data, particularly if they are to be used for automatic zero or span corrections. However, data should not be rejected to hide instrument drift problems.

#### 4.3.6 Enter or Calculate Span and Zero Correction Parameters

The appropriate zero and span corrections for all the DAS channels need to be in the “Corr Zero” and “Corr Fac” columns in the “Data Channel Control” sheet in order for the processed data to be properly corrected and calibrated. The appropriate procedure for deriving and entering these corrections depends on the instrument or data channel involved. There are essentially four categories of instruments or channels in this regard:

0. Those where no correction is appropriate;
1. Those where the corrections are essentially constant;
2. Those where corrections vary sufficiently slowly over time that they should be derived based on long-term trend data, usually using results of calibrations that are carried out separately from the experiments; and
3. Those where the zero and/or span corrections vary sufficiently from run to run that they are best derived from zero and/or span data for each experiment.

Note that in some cases the zeros and spans may be classified differently in this regard, e.g., an instrument where the span varies infrequently but the zero is highly variable would be category “3” for zero and “2” for span. The appropriate categorization in this regard should be specified in the SOP for the instrument and also entered in the “Zero Meth” and “Span Meth” columns in the “DAS Connections” sheet of the Instrument Information File (InstInfo.xls).

The appropriate procedures that should be used for entering or deriving the span correction factors for each of these categories are described below.

Category 0 and 1: Constant or No Corrections. In these cases, the default zero or span corrections (which should be 0 and 1, respectively for Category 0) should be in the template and should not be modified. If the correction parameters in the template are inappropriate, then the Data Processing Manager should be informed that the template needs to be corrected. The correction parameter value should be given with the SOP for the instrument and also entered in the “Default Zero” and/or “Default Span” column in the “DAS Connections” sheet in InstInfo.xls. If the channel is not in the template, then the appropriate corrections for the run should be taken from there and entered into the appropriate columns in the “Data Channel Control” sheet in the run data file.

Category 2. Externally-Derived Corrections. In these cases, the appropriate zero and/or span corrections for the time period of the experiment should be taken from the instrument’s log book or calibration database file and entered manually for each experiment into the “Corr Zero” and “Corr Fac” columns in the “Data Channel Control” sheet. The value in the template should not be used unless it is verified that it is the same as the currently assigned value, or unless the calibration SOP includes updating the corrections in the template. In some cases the final correction parameters may be derived based on trend data that will include data from calibrations made after the experiment, in which case the parameters in the run file may need to be updated and the processed data recalculated once they are determined.

In all the above cases the “Use Auto Zero” and/or “Cal Source State” columns should be blank so the default or manually entered values will not be over-written if the “Auto Zero Span” macro is run. However, results of zero and span checks during the experiment are useful for quality control purposes, and depending on the SOP for the instrument it may be appropriate to track the run to run span and zero results. If significant discrepancies are found then the need for re-calibration or other corrective action is indicated. However, it is inappropriate procedure to apply run-to-run corrections for channels in categories 0 - 2.

Category 3. Run-to-Run Corrections. For category 3 channels, the appropriate procedure is to use the auto zero or calibrate procedures to derive the correction factors if the necessary zero or span data are available and of satisfactory quality. If run-to-run zero corrections are appropriate, then a “yes” should be entered in the “Use Auto Zero” column in the “Data Channel Control” sheet. If run-to-run span corrections are appropriate then the formulas to obtain the appropriate span state and concentrations from the data in the “Cal Sources” sheet should be entered in the “Cal Source State” or “Cal Source Conc” columns in the “Data Channel Control” sheet. The template should already have appropriate entries in these columns if this is a usual channel for these experiments.

The concentrations in the span sources should be entered as appropriate in the “Cal sources” sheet, the time this concentration was derived or last verified should be entered in the “Date Last Checked” column, and other applicable documentation information should be given in the “Other Cal Source Documentation Information” sheet. The values in the template should not be relied upon as being correct without checking, unless the calibration or span source SOP calls for updating the template when the current span values change. In the latter case, the template should include the documentation for the values entered.

The “Auto Zero Span” macro, accessed by a control on the “Data Channel Control” sheet, is used to derive the zero and span corrections that give the desired average concentrations in the zero and span states for the applicable channels. Before running this macro, it is essential to complete the entry of all the sample state corrections and bad data flags that may affect the zero or span data that are used, and to verify this by examining the plots of these data, as described in the previous section. Note that if a number (which should be at least 3) is entered in the “Reject n x Sdev” column in the “Data Channel Control” sheet then points that are 3 or more standard deviations from the averages in the states are not counted when computing the average. In those cases, a few clearly anomalous points will not affect the results.

The results of the Auto Zero Span” calculation should be checked by first examining the averages for the zero and span states in the columns for them in the “Data Channel Control” sheet, then by looking at plots of the zero and span data for the affected channels. The affected data should be distributed about zero or the desired span values if the procedure operated correctly and if bad data did not affect the results.

If there are insufficient data to compute the zero or span corrections for a category 3 channel or if the data are of sufficiently low quality that an estimated correction would have less uncertainty, then estimated corrections would need to be applied. These could be derived based on results of other experiments carried out around the same time which had good span data, or on results of recent calibrations. The need to use estimated factors for these channels should be entered in the “Comments” column in the “Data Channel Control” sheet, and the data are of high priority for the run a comment about the correction uncertainty should also be entered in the “General Comments” section of the “Log” sheet.

**IMPORTANT:** The checklist entry “Check ‘Data Channel Control’ sheet for appropriate span and zero correction parameters” should NOT be checked unless the ALL the corrections have been verified to reflect the best available data or estimates, and derived using the appropriate procedures discussed above.

#### **4.3.7 Enter GC Data**

The “GC Data” sheet is used to enter all the GC data and calibration factors, which presently must all be entered manually. Eventually new data processing macros will be developed to load in the GC data from the HPCHEM files, but this has not yet been implemented. The procedures for manual entry are indicated below.

All species and instruments used for the GC measurements should be listed on the “Sampled Compound List” section, and the appropriate calibration factor given. The species names used should be standard Chadpro species names, as listed in the Species Information File (ExptSpec.xls) and the GC instrument IDs should match those given in the “ID” column in the “GC Instruments” sheet in InstInfo.xls. The current calibration factor should be entered in the column provided. If the factor is preliminary or uncertain a comment should be included in the “comments” column indicating that fact. If the factor is unknown then a “1” should be entered in the “factor” column, and a comment indicating it is raw data should be entered.

The template may already contain lists of compounds and instruments in the Sampled Compound List section. These should be retained even if there are no data of this type in this run because some of the modeling files may expect them in this order. Additional species/instrument combinations that are needed can be added after these, with lines being inserted as needed if the available space is not sufficient. In this case, formulas in the columns with calculated data (indicated by blue font) should be copied to the new rows.

The results of the individual measurements are entered in the “GC Data For Run” section. The state code indicating where the sample was taken (usually a reactor state) should be given in the “Code” column, with the numbers being the same as used for the DAS channels. An “x” can be entered in that column if the sample is known to be bad, in which case a comment indicating why the measurement was rejected should be entered in the space provided. Note that the “conc” column has a formula to calculate the concentration from the raw data entered in this section and the factor entered above, and if the cell in that column is blank it should be copied from another row in this section. If the instrument and compound name does not exactly match those given in the Sampled Compound List section, then a “#N/A” will appear in the concentration column. In this case either correct the spelling for the species or instrument, or add the species/instrument combination in the sample compound list. If there is insufficient space for all the data in the space provided, add rows as needed and copy the “conc” formula from other rows to the new rows.

The “Process GC Data” macro will copy the calculated concentrations to the processed data sheets for the appropriate states, and also place calculated initial concentrations for the reactor states for the species/instrument combinations in the columns provided for them in the Sampled Compound List section. An “ok” will appear in the “ok” column for each line in the “GC Data for Run” section where the data were successfully processed.

At present there is no plotting capability implemented to view GC data. This will be added later when needed. However, the processed GC data can be examined on the sheets for the individual sampling states. Note that the columns of GC data come after the columns of DAS data, so generally the GC data column numbers may be relatively high. The processed GC data columns are in the order they are listed in the Sampled Compound List section, in the same sets of columns for each sheet. If there is no GC data for a particular species/instrument combination for a particular state, the sets of columns assigned to it are empty. (This is also the case for the data in the DAS channels.)

#### **4.3.8 Enter Injection Information in the “Injections” Sheet**

The “Injections” sheet that was moved or copied from the Run Instructions file to the Run Data file contains a series of columns labeled “Injections as Achieved” that need to be filled in to reflect the injections that were actually made during the experiment, and the resulting concentrations. Some of this information can be filled in at the same time the other run documentation and comments are being entered from the log book, but others require completion of the processing of the measured data before they can be entered.

The times the injections began and ended and the amounts injected and information necessary to relate these amounts to concentrations in the reactor should be entered in the space provided. The appropriate entries for the amounts injected and related columns will depend on the injection method used. Examples of the types of information that should be provided for representative types of injection methods are indicated below.

<u>Injection Type</u>	<u>Amount Injected</u>	<u>Injector Volume</u>	<u>Other Information Needed</u>
Liquid	Microliters of liquid	N/A	Density and molecular weight
Gas (Vacuum system)	Torr in injection bulb	Liters of bulb	N/A
Gas (Syringe)	MI gas	N/A	N/A
Perm source	Concentration in source output	Calculated source volume	Source flow rate and injection time

In addition, the formula to calculate the “amount injected” column should be entered in the column provided for it, using reference to the cells containing all the data used to make the calculation. Other than metric conversion factors indicating changes in orders of magnitude (e.g., ml to liters, etc.), formulas in chamber data processing spreadsheets should NEVER contain numbers. If a number is needed that is not in the sheet, then it should be added at an appropriate location in the sheet, and labeled accordingly. Common conversion factors and space for entering the temperature and assumed chamber volume are provided in the sheet, and should be used when needed. The template has formulas for calculating amounts injected for some common injection methods, which can be copied to rows where such injection methods are used.

Most of the calculations of the amount of compound in the reactor from amounts injected require the volume of the reactor, which may be uncertain. The cell labeled “Reactor Volume Used to Calculate Concentrations” should have the measured or estimated volume that is used in the calculations in the formulas in the “Calc Conc” column. The cell below it, labeled “Reactor Volume Used to Determine Injection Amounts” should have the volume that was used by the experimenters when calculating how much of each compound to inject before the experiment began. The cell below that, labeled “Calculated Reactor Volume After Injections” is available for giving the revised reactor volume estimate based on the measured concentrations in the experiment. If there is more than one reactor and it is not assumed they have different volumes, the cells to the right can be used for the volume estimates for the additional reactor(s), and the formulas referring to the reactor volume should be modified to refer to the appropriate cell for injections into those additional reactors.

If there were any problems or special procedures applicable for a particular injection or set of injections, then a footnote code should be entered in the “Notes” column, and comments describing the problem or procedure should be entered in the space provided for footnotes below the injection amounts table.

Once the data are processed at least to the extent that the initial concentrations of the injected species have been computed, the initial concentrations should be entered into the “Meas Conc” column. These would come from the “Initial or Average Data” columns for the appropriate reactor in the “Data Channel Control” sheet for compounds measured using DAS channels, and in the “Initial Conc” column for the reactor in the “Sampled Compound List” of the “GC Data” sheet for species measured by GC. If there is more than one measurement, the average concentration from the highest priority instruments should be used.

#### **4.3.9 Other Data Relevant to Experiment**

For some experiments, there may be special measurements or other types of data taken that are not processed in the same way as the DAS or GC channels. If these types of measurements become routinely associated with these experiments, then the data processing procedures and templates should be modified to account for them, and the associated SOP's and data processing instructions should be updated accordingly. In the meantime, worksheets containing the additional data in appropriately documented format should be added to the run data file, and comments should be added to the General Comments section in the "Log" file about the existence of the additional sheets and data. The Project Scientist should add appropriate entries to the Checklist and Instructions for the experiment to assure proper processing of these data, if needed.

#### **4.3.10 Preparation of Data for Modeling**

A full discussion of the procedures for preparation of data for modeling is beyond the scope of the present document. Briefly it requires that the data be processed completely as discussed above, or processed at least to the extent that the processed data incorporate current best estimates for all correction factors used, and inappropriate data for reactor states have been removed. Most of the modeling preparation involves making appropriate entries in the "Model Input" sheet, and using the macros accessible there to produce the modeling files required.

#### **4.3.11 Final Disposition**

The post-experiment data processing operations discussed above should be carried out as soon as practical after the experiment has been completed. However, the data in the experiment may not be finalized until some time afterwards because some corrections and model input parameters may require examination of trends involving measurements and calibrations made after the run. The Project Scientist should determine a reasonable time to finalize the data for an experiment, at which time all the factors and model input assignments used should be reviewed and if appropriate modified. If changes are made, the data should be re-calculated and any modeling input files produced previously should be re-generated. Only after this is done should the "Correction Factors Finalized" and Model Input Finalized?" items on the checklist be checked off.

The run data file and the raw data files that it uses should be archived after the completion of the run and the run data file is completely filled out. They should be archived again after the run is finalized. The data archiving procedures are described in the data archiving SOP, which is in preparation. This will include maintenance of a archive log file that will include a sheet listing all experiments and the date and media ID for the last archive of their data.

## **5 Backups and Archives**

### **5.1 Backups**

Computer storage systems fail from time to time and backups of critical files are needed to minimize the disruption and loss caused by such failures. Although the CE-CERT computer operations personnel attempt to back up PC's connected to the CE-CERT network at regular intervals, in practice this has not been consistent or reliable, and should not be counted on for critical files. Although the CE-CERT network of Unix computers is expected to have more reliable backups in the near future, consistent reliability has not yet been assured. For that reason, personnel working on this project should *not* assume

that backups of critical files exist unless steps are taken by them. Minimum steps that should be taken are discussed below.

At a minimum, copies of all critical files for this project should exist on at least two computers, preferably in different buildings and locations. New or changed files should be copied for backup purposes at least once a week, or whenever the file represents at least eight person-hours of labor, whichever is more frequent. Steps to assure this, and personnel responsible for these steps, are as follows:

- Files for this project on desktop computers of staff members should be copied to the APL group shared disk on the CE-CERT Unix network at least once a week, unless an acceptable alternative backup arrangement is made. Each staff member using this backup method should create a subfolder with his or her name in \\ozone\backups and copy the files there using the same directory structure as exists on his or her computer. If the computer has more than one partition, the directory structure should start with the drive letter. For example, a file D:\projects\EPAcham\my-data-workup.xls should be copied to \\ozone\apldata\backups\person\D\projects\EPAcham\my-data-workup.xls, where “*person*” is the name of the staff member. The Quality Assurance Officer is responsible for seeing that this is enforced.
- An alternative approach is to copy all new or changed files to a removable portable disk drive and then copy those files to the staff member’s home computer at least once a week. Files that represent more than 8-hours of work can be copied to the portable drive without having to go home, so at least the file will exist in two locations. This is the approach used by the Principal Investigator for this project. Permission from the Quality Assurance Officer is required for other staff members to use this method in lieu of copying the files to \\ozone\apldata\backups.
- Files containing collected data on instrument-dedicated computers should be copied either to an appropriate folder in \\ozone\apldata\instruments or \\ozone\apldata\backups at least once a week when the instrument is in operation. The operator of the instrument is responsible for seeing that this is reliably carried out. The SOP for the instruments should include a provision for this operation, and indicate the exact locations for the backups.
- The changed and new files on \\ozone\apldata and \\ozone\apublic will be copied to a portable hard disk and then copied to a designated staff member’s home computer at least once a week. This will continue until the consistency and reliability of the CE-CERT Unix backup system has been assured, and there is a plan for storing the backup media in a separate location from CE-CERT. The designated staff member (currently the Principal Investigator) will be responsible for seeing that this is carried out.

Note that copying data from \\ozone\apldata to \\ozone\aplshared is *not* an acceptable backup approach because not only are these two shares on the same computer, they are also on the same physical disk. An acceptable backup at a minimum must be a different computer and disk and preferably also a different building.

Staff members are also encouraged to back up critical files periodically on CD-ROM or other appropriate media. Before any backups are considered to be complete, the ability to read the data from the media *on another computer* should be verified. If a removable backup device is used to make the backup, a different device should be used to verify the backup. Other than that, required standard procedures and frequencies for making such backups have not yet been established.

## 5.2 Data Archives

Data archives differ from backups in that they preserve files that may be changed or no longer needed online in a consistent basis. It is the responsibility of the Principal Investigator and the Quality

Assurance Officer to see that appropriate archiving procedures are carried out, or to delegate these responsibilities to the appropriate personnel. The minimum archiving procedures that should be followed are as described below

Non-rewritable CD-ROM should be used as the archive media, with the data recorded in a format that can be read by conventional PC CD-ROM drives. Alternative media may be considered, but to be acceptable they must be reliable and a well-established format that will persist into the foreseeable future, and readable on computers that are widely used. Tape media and media with proprietary formats are not considered acceptable for archiving purposes.

Only CD-ROM software that has the capability to verify successful copies by comparing files on the CD with files on the source disk should be employed, and the option to do this should be selected. Re-do the backup if problems are encountered. Once the backups are completed, each CD-ROM should be verified for readability using another CD-ROM drive on another computer.

The CD-ROMs should be labeled with the date, the computer, share, or runs being backed up, and folder or files involved, as applicable. If multiple CD's are required, they should have the number of the CD and the total number (e.g, "2 of 4"). The CD disk itself should be marked as well as the label cover (if it is the type that can be marked) so it can be identified if it is separated from the label.

A log book for archives will be created and stored in the "manager's" office in the AP laboratory building or near the computer to be used for making the CD backups. All archives, backups and ID labels of the CD-ROM or other media used, and the locations where they are stored, will be noted in that book when they are made.

As indicated above, two sets of archive CD backups should be made. One set should be stored at an assigned location or file at CE-CERT to be determined. The other set should be stored at a different location also to be determined. For the time being, the location at CE-CERT will be the bookshelf near Bill Carter's office where the old lab books and lab book copies are stored, and the remote location will be Bill Carter's home.

### **5.2.1 Working file archives**

At least twice a year, once just before the Fourth of July holiday and once before the Christmas break, two complete sets of CD-ROM backups of all files on \\ozone\apldata and \\ozone\apublic. Before these backups are started, all staff using \\ozone\apldata to back up files on their desktop or instrument PCs should update their files in their backup folders, so the archive contains the most up-to-date files for the PCs that are being backed up using this disk. Only non-rewritable CD media should be used for this purpose, since the intension is to archive the data.

If any other computers are used for this project whose data do not exist on \\ozone\apldata or \\ozone\apublic, either as the primary version or backups, complete archives of all folders on those computers containing project data should also be made. These should be made at the same time as the working file archives, i.e., just before the Fourth of July and the Christmas Holidays.

Because all the files in the partitions being backed up will probably not fit in a single CD-ROM media, steps should be taken to assure that all files are backed up and that nothing is missed in the process of backing up to multiple media. A SOP to accomplish this should be compared.



### 5.2.2 Run Data Archives

Separate archives of raw and processed data from EPA chamber runs will be made at appropriate intervals once the data for a series of runs have been completely processed, or whenever reports describing the data are finalized. The archiving of these runs will be noted in the backup/archive log book so the latest archive data from a given run can be located if they are not available on line. Once the data from a run are archived they do not need to be re-archived unless modifications or additions to the data are to be made, or the data are to be deleted from the on-line disks.

The archives should be made by creating a temporary folder and making sub-folders within that for each run to be archived. All the raw and processed data files for that run should be copied into that folder, using subfolders for different types of data if necessary to avoid confusion as to which raw data file is which. Note that this includes raw data of all types from all instruments used as well as the data logger outputs for the period of time that the run was conducted. This includes TDLAS and LiCor spectra and GC data files. Note also that in some cases a particular raw data file may span the period of more than one run, in that case that raw data file should be copied into the folder for all the applicable runs. A convention of directory structures for archives should be established and documented in the archive log book, and this should be followed for all run data archives. A SOP document for creating such archives should be prepared (at present such as SOP does not exist.)

A separate set of archives of the run data should be made before any of the data from the run, including raw data files, are deleted from the on-line disks. No deletions should be made unless at least two backup copies have been made, and the files on at least one of the backup media have been compared with the files to be deleted.

The time and locations of the run data backups should be noted in the appropriate column of the master run listing file, which is currently \\ozone\apldata\chambers\actruns.xls. (If a column indicating this information does not exist for the particular series of runs it should be created.) Separate columns should be used to indicate the date and the label that the latest archive for the run data was created. If new archives are created, this should also be indicated.

## 6 Tables

Table 1. Summary of personnel and responsibilities for UCR EPA environmental chamber experiments.

Designation	Description of Relevant Responsibilities	Personnel (primary, backup)
Project Scientist	Ultimate responsibility for project for which experiment is conducted. Gives instructions for how experiments are to be conducted and priorities for data acquisition and processing. Ultimately responsible for assuring that the proper procedures are followed.	Bill Carter, Dennis Fitz
Data Processing Manager	Responsible for establishing the data processing procedures, data processing file formats, and data processing programs and macros.	Bill Carter, (primary backup to be determined)
Quality Assurance Officer	Responsible for quality assurance for the overall project. Conducts periodic audits to assess whether appropriate procedures are followed on an ongoing basis, and makes recommendations when corrective action is needed.	Dave Gemmill, Dennis Fitz,
Primary Run Technician	Overall responsibility for a particular experiment being conducted as requested by project scientist. Overall responsibility for seeing that all relevant data, calibration information, experimental parameters, and documentation are entered in the appropriate manner in the run data file. Responsible for completion of the data processing checklist for an experiment in a timely manner. Responsible for assuring that the run data file and log books appropriately document the operations carried out during the runs. Note that each experiment will have only one Primary Run Technician, though the person who has this responsibility may vary from run to run.	Irina Malkina, Kurt Bumiller, Claudia Sauer
Primary Instrumentation Technician	Responsible for proper operation and calibration of all instruments that are not the specific responsibility of another instrumentation technician. Responsible for maintaining and keeping up-to-date any calibration databases associated with these instruments. Responsible for the proper operation of the sampling and on-line data acquisition systems. Responsible for assuring that the master files giving the current instruments used, connections, and sampling state information always reflect the current configuration. Responsible for assuring that the run data file appropriately represents the instruments, connections, and sampling states used for the run.	Kurt Bumiller, (primary backup to be determined)

Table 1 (continued)

Designation	Description of Relevant Responsibilities	Personnel (primary, backup)
Specific Instrument Operator	Responsible for the proper operation and calibration of a particular instrument or set of instruments. Responsible for maintaining and keeping up-to-date any calibration databases associated with these instruments. Responsible for assuring that the run data file has quality-assured data and relevant calibration data and other parameters needed for properly processing the data. Responsible for assuring that the documentation in the run data file appropriately reflect any problems that may affect the quality of the data from the instrument(s).	TDLAS's: Claudia Sauer, John Pisano GC's: Irina Malkina, Claudia Sauer AO HCHO: Claudia Sauer, Kurt Bumiller NO2-GC's: Kurt Bumiller, Dave Pankratz
Run Modeler	Responsible for assuring that the conditions of the experiment are properly represented for modeling. Inputs run specific model input information where appropriate in run data file. Maintains characterization files associated with particular types of experiments based on results of analysis if characterization data.	Bill Carter, (backup to be determined)

Table 2. Summary of computer files used for environmental chamber experiments.

Designation	Name	Network Location	Description	Responsible Personnel
<u>Run Data Processing Files</u>				
Run Instructions File	RunInstr.xls	\\ozone \apldata \chambers	File containing instructions for runs to be carried out. Contains a summary of the runs desired and sheets containing instructions, injections worksheet, and checklist for individual runs that are moved to the run data file when the run is completed.	Project Scientist  Primary Run Technician
Run Instructions Template	NewInstr.xlt	\\ozone \apldata \chambers \templates	Template used to create a the run instructions, reactant injections, and checklist sheets for a run, which are then moved to RunInstr.xls	Project Scientist
Run List File	Actruns.xls	\\ozone \apldata \chambers	Contains a log of the runs carried out and brief comments on special problems or operations.	Primary Run Technician
Run Data File	<i>runid</i> .xls where ' <i>runid</i> ' is the run designation [a]	\\ozone \apldata \chambers \runfiles	Excel file that contains the raw and processed data from each experiment, as well as run-specific comments and parameters that are needed for documentation. A separate run data file is created for each experiment. Contains multiple sheets with different types of data and information. Described in detail in the "Run Data File" section, below.	Primary Run Technician  Run Modeler [b]
Run Data Template	EPAdata.xlt	\\ozone \apldata \chambers \templates	Excel template file used as the starting point for the run data files. In addition to containing the template for the sheets where the run specific data will be input, it contains default parameters used for current experiments.	Data Processing Manager
Run Data Control and Plotting	EPApplot.xls	\\ozone \apldata \chambers	Excel file containing the macros used when processing the data in the run data files. Also contains plots of the data in the run data file currently being viewed and processed. Normally this is loaded into Excel along with the Run Data file. The contents of the file is described in the "Run Data Control and Plotting" file section, below, and the use of its macros are described in the "Data Processing Procedures" section.	Data Processing Manager  Primary Inst. Technician [c]

Table 2 (continued)

Designation	Name	Network Location	Description	Responsible Personnel
Current Data File	EPAdata.xls	\\ozone \apldata \chambers	A special type of Run Data file that can be used to view plots of data from currently ongoing experiments, or from previous selected days, regardless of which run they are associated with.	Data Processing Manager
Control parameter file	ChamWork.xls	C:\Chadpro (on each computer used)	Contains information needed to use the run data control and plotting file in a particular computer. Also can be used to conveniently load and use the run data and data control files from any computer where it is installed.	Data Processing Manager
<u>Configuration and Documentation Files</u>				
Valve State Control File	Valves.xls	\\ozone \apldata \chambers	Contains information defining what is being sampled for each set of valve configurations. Contains definitions of named sample states. Contains definitions of named sampling schedules and macros to output these schedules in a format that can be used by the valve control program for the sampling system.	Primary Inst. Technician  Data Processing Manager [d]
Instrument Information File	InstInfo.xls	\\ozone \apldata \instruments	Contains descriptions of all instruments currently employed by the CE-CERT AP group, their model and serial number, and the designation used for each in the run data and other data processing files. Indicates data output by each (except for GC instruments). Also information on how the instruments are interfaced to the data acquisition system, and which data acquisition channels and channel names are used for each connected instrument.	Primary Inst. Technician  Data Processing Manager [d]
Species Information File	ExptSpec.xls	\\ozone \apldata \chambers	Contains list of all species and physical parameters that are (or might be) monitored in chamber experiments. Can be used to assure that Chadpro standard names are used measured species or parameters	Project Scientist  Data Processing Manager
GC Calibration Information File	Gccal.xls	\\aplpc3 \chadpro	Contains calibration history and current calibration assignments for all GC instruments (NOT YET IMPLEMENTED)	GC Inst. Operator

Table 2 (continued)

Designation	Name	Network Location	Description	Responsible Personnel
Instrument Calibration Information Files	<i>instid.xls</i> [e] [x]	To be determined [y]	Contains current calibration history and current calibration assignments for all non-GC instruments where this is appropriate (NOT YET IMPLEMENTED)	Primary Inst. Technician or Inst. Operator
<u>Raw or Primary Processed Data Files</u>				
Primary DAS raw data files	Dmmdyy.Csv [f]	\\blackhole\data\1M	Primary data output from the data acquisition system containing data from all instruments connected to the system. Data read into the run data file using the macros in the run data control and plotting file. A separate file is created for each day. Format discussed in the “Data Processing Programming Information” section.	Primary Inst. Technician
Valve State Files	Vmmdyy.txt [f] [x]	\\blackhole\data\valves	Output by the valve control program to indicate the state of all the valves and flags as a particular time. Data read into the run data file using the macros in the run data control and plotting file. A separate file is created for each day. Format discussed in the “Data Processing Programming Information” section.	Primary Inst. Technician
Raw Analog Data Files	Ammddy.csv [f] [x]	\\blackhole\data\analog	Raw analog data output by the data acquisition program. A separate file is created each day. Not used for current data processing, but retained for archiving.	Primary Inst. Technician
Raw Serial Data Files	Smmddy.csv [f, g] [x] (Current format is <i>Smmddy 0c.csv</i> )	\\blackhole\data\serial	Raw serial data input to the data acquisition program. A separate file is created each day. These are currently used as the primary means for inputting raw data from the TDLAS instruments (c=5 or 6 for TDLAS#1 and TDLAS#2, respectively), but not for other instruments with serial connections to the system.	Primary Inst. Technician
Raw TDLAS Data Files	Controlled by TDLAS software [h]	\\ozone\apldata\instruments\TDLAS\RawData\tdl_yymm [i]	Copies of output files produced by TDLAS programs. Separate files are created for each TDLAS channel for each day for various types of data. The PRN files contain the measurement data that can be read into the run data file using macros in the run data control file. These are currently not used for data processing but are retained for archiving purposes.	TDLAS Instrument. Operator

Table 2 (continued)

Designation	Name	Network Location	Description	Responsible Personnel
Processed TDLAS Data Files	<i>species-runid.xls</i> [a, j]	\\ozone\apldata\instruments\TDLAS\species [j]	If manual processing of the TDLAS data is required before it is acceptable for use in the experiment, these files contain the processed data for the run, with a separate file for each TDLAS channel. These data are then read into the run data file using the macros in the run data control file. The data in these files must be formatted so they can be read by these macros, as discussed in the “Data Processing Procedures” and the “Data Processing Programming Information” sections. These files may contain additional data, plots, etc. that the operator may feel appropriate for processing or documenting these data.	TDLAS Instrument Operator
GC Data Files	Controlled by the GC HPCHEM software [k]	\\aplpc3\c\HPCHEM\n\data\runid\hmm.D [a, k]	These files are produced by the HPCHEM GC software whenever GC samples are taken. The chamber data processing macros will eventually be used to read these files and input the GC data into the run data files. (Not yet implemented.)	GC Instrument Operator

- [a] The run designation contains a two- or three-character prefix indicating the chamber (“EPA” for EPA chamber runs) and a three-number designation giving the run number. For example, for the third experiment conducted in the EPA chamber, *runid* is replaced by “EPA003”.
- [b] The run modeler is responsible only for the “Model Input” sheet. The Primary Run Technician is responsible for all other sheets except for those created by the data processing macros.
- [c] The Primary Instrumentation Technician is responsible for assuring that the Data Processing Manager implements the correct macros for computing the appropriate sampling state from the valve state flags output by the data acquisition programs.
- [d] The data processing manager is responsible for establishing the format of the files and the proper operation of any macros they may contain. The primary instrumentation technician is responsible for assuring that the information in the files is correct, complete, and up-to-date
- [e] “*Instid*” is the Chadpro instrument designation number as indicated in the InstInfo.XLS data set.
- [f] The characters “mm”, “yy”, and “dd” refer to the month, day, and year as two-digit numbers. I.e., for files with data for March 13, 2002, “mmddy” is replaced by “031302”.
- [g] The character “c” refers to the serial channel number, in a base-36 numbering system (i.e., the letters “A”, “B”, ... “Z” etc. are used to refer to channels 10, 11, ... 35.)
- [h] PRN, HAV, and QAV files are produced for each TDLAS channel and day of measurement as discussed in the documentation for the TDLAS instrument. The file names have the format chddMMn, where “ch” indicates the type of measurement (FM for formaldehyde, HP for H<sub>2</sub>O<sub>2</sub>, NO for NO<sub>2</sub>, and NA for nitric acid), “dd” is the numeric day number, “MM” is a two-character month code (JA, FE, MR, AP, MY, JN, JL, AU, SE, OC, NO, and DE), and “n” is the channel number.
- [I] The characters “mm” and “yy” refer to the month and year as two-digit numbers. I.e., files with data for March, 2002, are located at \\ozone\apldata\instruments\TDLAS\rawdata\tdl\_0203.

Table 2 (continued)

- [j] "*Species*" refers to the species being measured by TDLAS, and is replaced by "NO<sub>2</sub>", HNO<sub>3</sub>", "HCHO" or H<sub>2</sub>O<sub>2</sub>" as appropriate.
- [k] The files produced by the HPCHEM software is described in the HPCHEM documentation. The GC data are stored under the HPCHEM directory using the directory structure indicated, where "*n*" refers to the HPCHEM instrument number, "*hhmm*" refers to the 24-hour clock time in hours and minutes, and *runid* is the run designation. This convention must be followed for the data processing programs to be able to find the data for a given run.
  
- [x] This naming convention has not yet been implemented for this type of file.
- [y] This file location has not yet been implemented.



Table 3. Preliminary version of the "Instructions" sheet in the Run Instructions template

**Instructions for EPA Chamber Experiment**

(Project Scientist's Instructions in Black) (Experimentalist's Modifications and Notes in Red)

Preliminary Run ID: \_\_\_\_\_ Final Run ID: \_\_\_\_\_

Run Title: \_\_\_\_\_

Purpose: \_\_\_\_\_

Project Scientist: Bill Carter

Primary Run Technician: \_\_\_\_\_

Instructions Date: \_\_\_\_\_

Desired Run Date: \_\_\_\_\_

Reactor Preparation	Requested	Achieved
Dumps and Fills:	_____	_____
Purge time:	_____	_____
Mixing Time:	_____	_____

Other Reactor Preparation Instructions

\_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_

Injection Instructions (see "Injections" sheet for details on amounts)

\_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_

Sampling and Span Schedules (Indicate modifications from instructions in red)

Sampling Schedule (minutes in state)						Spans	
Sampling State	Before Injections	Before Lights	First Hour	Rest of Run	After Run	Type	Frequency
Zero Air						NO	
Reactor A						O3	
Reactor B						GPT	
Enclosure							
Spans							

Other Sampling Instructions

\_\_\_\_\_  
 \_\_\_\_\_

Priority Measurements

_____	_____
_____	_____
_____	_____

Other Instructions

\_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_

Instructions as Actually Implemented (if followed exactly, indicate that this is the case)

\_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_



Table 5. Preliminary version of the data processing checklist for EPA chamber experiments

**DATA PROCESSING CHECKLIST FOR EPA CHAMBER EXPERIMENT EPA-000**

Run ID: EPA-000  
 Run Date: .....  
 Run Title: .....  
 Project Scientist: .....  
 Primary Run Technician: .....  
 Primary Instrument Technician: .....  
 GC Operator: .....  
 TDLAS Operator: .....  
 Other Operators: .....  
 .....

---

**PROCESS RUN INSTRUCTIONS**

---

Run Instructions Reviewed and Accepted by Run Technician .....  
 Sampling Schedule Programmed to be Consistent with Instructions .....  
 Comments entered on run instructions sheet to reflect any modifications. ....  
 (use Red font for edits) .....  
 Modified instructions accepted by project scientist (if applicable) .....

---

**LOG RUN**

---

Run number entered on summary sheet of Run Instructions File .....  
 Run number and description entered on "Run List" file .....  
 If problems or special operations occurred that should be included in the run list file, have  
 they been included in the appropriate column there? .....  
 If the extent with the operations as actually implemented differ from the instructions  
 appropriately indicated on the "Instructions" sheet? .....

---

**CREATE AND INITIALIZE RUN FILE**

---

Run File Created and Correct ID number entered on Log sheet .....  
 Instructions, Injections, and Checklist Worksheets Moved from Run Instructions  
 File to the Run Data File. ....  
 If run is considered to be unsuccessful, then the Instructions, Injections, and Checklist  
 worksheets should not be deleted from the Run Instructions File.  
 Is this the case for this run? .....  
 Are the "Side ID"s for all the reactor states (or chamber "sides") that are used properly  
 indicated on the "Sampling States Code" section of the "Log" sheet and is there a  
 Chadpro file name for each? .....

Table 5 (continued)

<b>ENTER COMMENTS AND EVENTS IN LOG SHEET</b>	
	<b>Enter Major Run Times</b>
Time zone indicated correctly (standard or daylight)?	.....
Data start and End times	.....
Lights On time	.....
Lights Off Time	.....
Time Bag Filled	.....
Time Injections complete and mixed	.....
	<b>Check Sampling State Codes Section</b>
All sampling state codes and descriptions appropriate?	.....
Sampling State Stabilization Times Appropriate?	.....
Is there a Chadpro Output file specified for each experiential reactor (or chamber side) used?	.....
	<b>Fill In Event Log Information from Log Book:</b>
Major operations entered	.....
Problems or observations entered	.....
Manual sampling states for main sample line entered	.....
	<b>Fill out "Offline or Non-Standard States for Selected Channels"</b>
All times instruments offline or giving bad data entered	.....
Times other sample inlet lines have different sampling states	.....
<b>ENTER INJECTION INFORMATION IN "INJECTIONS" SHEET</b>	
Reactor volume used when calculating injections entered	.....
Injection times, method, amounts injected, etc. entered	.....
Formulas entered or copied for computing amounts injected and results checked for reasonableness	.....
Comments entered concerning any injection problems or procedures	.....
<b>PREPARE TO LOAD DAS DATA</b>	
Does the "Sample Inlet Control" sheet correctly specify the sampling setup?	.....
Are all files to be loaded specified correctly in the "Data File Control" sheet?	.....
	<b>Check the "Data Channel Control" Sheet</b>
Are all online channels listed?	.....
Are all instrument ID's correct?	.....
Is the "Sample Line Number" appropriate for each online channel?	.....
Are the Data Source File types and labels or columns correct?	.....
Are the Minimum and Maximum Data OK values appropriate?	.....
Are the Time Offsets and Stabilization Times Appropriate?	.....
<b>RUN MACROS TO LOAD DAS DATA</b>	
"Initialize" Macro Run ok?	.....
"Load DAS Data" Macro Run ok?	.....
Are all files loaded (Check "ok"s in "Data File Control" sheet)?	.....
Are all online channels loaded (check "Loaded Data" sheet)?	.....
Is full range of times loaded (check "Loaded Data" sheet)?	.....

Table 5 (continued)

<b>CHECK LOADED DAS DATA, FLAG BAD DATA, AND MAKE STATE CORRECTIONS AS NEEDED</b>	
(If problems are found, make corrections to states or flag unusable data as needed by adding appropriate entries to the "Event Log" and "Non-Standard States" sections in the "Log" sheet. Then run "Update Flags" macro and re-run "Process Data" macro, and check again.)	
<b>Run "Update Flags" (if needed) then "Process Data" Macros</b>	.....
<b>Use EPAplot.xls to examine plots for online channels</b>	.....
Are there garbage or bad points on the plots?	.....
Are all data in "zero" state actually zero data?	.....
Do all data in the "span" states for the species being span checked represent valid and stable readings?	.....
Do the "reactor" data have bad data or data not representing stable measurements in the appropriate reactor state?	.....
<b>ENTER CALIBRATION AND CORRECTION PARAMETERS</b>	
<b>Check and fill in "Cal Sources" sheet</b>	
All span types used represented and state numbers correct?	.....
Span concentration correct?	.....
Date of last span concentration checked entered?	.....
Log book location or file with span documentation entered in "Other Cal Source Documentation Information" section?	.....
<b>Check "Data Channel Control" sheet for appropriate span and zero correction parameters</b>	.....
"Cal Source State" entered for ONLY those channels for which automatic calibration corrections will be made	.....
"yes" entered in "Use Auto Zero" for ONLY those channels for which automatic zero corrections will be made.	.....
<b>Enter Factor and Zero Corrections in the "Data Channel Control" sheet for all other Species where corrections are needed for which autozero or autocal should not or cannot be used.</b>	
Appropriate number entered in "Corr Factor" or "Corr Zero" columns	.....
Footnote (not "A") entered in "Note" column to right of factor or zero column and documentation footnote entered in "Footnote" section at bottom of sheet	.....
"Cal Source State" and "Use Auto Zero" column clear for all channels where assigned factors or zeros entered	.....
<b>MAKE AUTOZERO AND AUTO CALIBRATE CORRECTIONS</b>	
<b>Re-Check plots of "zero" or "span" data to be used in autozero or autocal to be sure that only valid and stable data will be used</b>	.....
<b>Run "Auto Zero" span macro</b>	.....
<b>Check plots for appropriate zero and span results</b>	.....
<b>Were Manual zero or span corrections on channels for which autozero or autocal failed?</b>	.....

Table 5 (continued)

<b>ENTER GC DATA</b>	
<b>Check and Update "Sampled Compound List" in "GC Data" sheet</b>	
Are all measured species and instruments used on the list?	.....
Are the instrument IDs valid instrument IDs as listed in InstInfo.xls?	.....
Are the species valid Chadpro species names (check ExptSpec.xls if unsure)?	.....
Is the proper priority entered?	.....
Is the proper factor entered?	.....
<b>Entered Measured GC data in "GC Data for Run" section</b>	
Are all data entered?	.....
Is correct state code given for all entries?	.....
Is a valid calculated concentration in the "conc" column for all entries? (fill in calculation formula if blank, correct spelling of species or instrument ID or add species, instrument and factor to "Sampled Compound List" if zero or "N/A")	.....
Are comments entered for measurements where comments are appropriate?	.....
<b>Process GC data</b>	
Is "ok" in all rows in "GC data for run section"?	.....
<b>ENTER OTHER DATA AS APPLICABLE</b>	
<b>If other measurements made that are not provided for in run file spreadsheet, add separate sheets to the file with those data.</b>	
Are instruments and operators identified in all such sheets?	.....
Are the meaning of all the data columns or fields clearly indicated on the sheets?	.....
Are the necessary calibration factors or correction factors applied?	.....
<b>ASSIGN INITIAL REACTANT CONCENTRATIONS</b>	
Is the time entered for "Injections complete (reactants stabilized)" on the Log sheet appropriate for computing initial (pre t=0) concentrations?	.....
Are initial concentrations given for the reactors of interest in the "Initial or Average Data" section of the "Data Channel Control" sheet for all the injected species measured using DAS instruments appropriate?	.....
Are initial concentrations given for the reactors of interest in the "Initial Conc" columns of the "Sampled Compound List" section of the "GC data" sheet for all the injected species measured by GC appropriate?	.....
<b>Measured initial concentrations of injected species entered in the "Meas Conc" column of the "Reactant Injections" sheet.</b>	
Copy calculated initial concentrations of species measured using DAS instrument of highest priority from the "Data Channel Control" sheet	.....
Copy calculated initial concentrations of species measured using GC instrument of highest priority from the "GC Data" sheet	.....
Fill in initial concentrations of other species based on available data for injected species that were not measured, and enter a comment on the "Reactant Injection" sheet saying how they were derived.	.....
<b>FINAL DISPOSITION</b>	
<b>Have data files been archived?</b>	
Run data file	.....
All raw data files	.....
Processed data files used for special instruments or other measurement data for run	.....
<b>Correction Factors Finalized?</b>	
<b>Run Conditions Set up for Modeling?</b>	
<b>Modeling input and output files reflect final correction factors and data?</b>	

Table 6. Description of worksheets and data in the Chamber Run Data Files.

Sheet and Designation	Purpose	Notes [a]
<u>“Log” sheet</u>	Gives major run documentation, parameters, comments, and event logs.	
Run ID	Run designation, .e.g., EPA $nnn$ , where $nnn$ is the run number. Automatically entered when the run file is created by “create new run” macro.	A, H
Run Description	Brief of the run, should fit into space provided without wrapping.	E
Purpose and General Comments	Purpose and general comments for the run. Generally entered by project scientist	F
Major Run Times	Gives time information used for loading or processing the data.	
Data Start Time	Earliest date and time for which data relevant to this run is collected. This together with the data end time determine which data are loaded.	A
Data End Time	Latest date and time for which data relevant to this run is collected.	A
Time Interval	Shortest time interval for data (minutes). Default of 1 minute should usually not be changed.	A, D
Time Initialized OK	The macro inserts an “ok” into this slot after the time array is initialized based on the specified starting and ending time. This “ok” should be deleted if the data start or ending times ever changed, so that the data processing macros will know that the time array needs to be re-initialized and the data need to be re-loaded for the new time array.	H
Time Zone	PST or PDT depending on time of year	A, D [b]
Time Bag Filled	Date and time the reactor was completely filled	C
Injections Complete	Date and time injections into the reactor(s) was completed and reactants can be assumed to be well mixed. This is used when computing initial reactant concentrations for modeling. If not given, the data processing procedures assume it is 30 minutes before lights on. Required for processing dark experiments.	C [c]
Time Lights On	Date and time the lights were turned on. Leave this and “Time Lights Off” blank if dark experiment.	C [c]
Time Lights Off	Date and time the lights were turned off.	C [c]
Minutes of Irradiation	Calculated number of minutes between time lights on and time lights off	F

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Sampling State Codes	This gives information concerning the different “sampling states”, i.e., sources of air being sampled, that may be involved with this experiment, such as reactor, zero air, calibration source, etc. The template defaults can be used in most cases except when the sampling configuration is different than indicated on the template.	
Sheet Name	The data processing macros output the processed data into separate sheets for each sampling state. This gives the name of the sheet used, and must not contain characters that are unacceptable in Excel sheet names.	B, D
Code	Numerical codes used to designate the various sampling states in the event logs (see below) and in other places in the file. Should be consistent with the state codes given in the Valve State Control File	B, D
Description	Description of the sampling state.	E, D
Stabilization Time	Number of minutes required for sampling from this state before useable data can be obtained. This is used if takes a longer time for the concentrations to equilibrate and reach stable levels than is case when sampling from other sources. Generally used for calibration sampling if it takes a while for the calibration levels to stabilize.	C, D [x]
Side ID	The code used to identify the reactor for this state if the data for this state are to be modeled. This should be blank for zero, span, or other non-reactor states. If this is a single reactor experiment, this should have the character “-“. If it is a dual or multi-reactor experiment, the reactor for state 1 should be designated “A”, and the others should be designated “B”, “C”, etc.	C, D [d]
Chadpro Output File	The file name to be used if data for that state are to be modeled. This consists of the side ID appended to the Run ID, or the run ID alone if the side ID is “-“.	G
Operations and Event Log	This is used to document the manual operations and major events associated with the run, and also indicate sampling states in those cases where they cannot be determined (or determined correctly) from the flags output by the data acquisition system. Note that these flags are applicable only to channels with “sample line” set at “1”, which is used to indicate that the sampling source is the main sample line (see discussion of the “sample line” parameter in the “Data Channel Control” sheet.	[e]



Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Date and time	Date and time of the event, or date and time that the manually input state <i>begins</i> . All times must be in ascending order or the data processing macros will abort with an error message. However, it is acceptable to have the same time as the immediately prior row.	C [f]
State	A blank in this column means that this entry is a comment for documentation purposes only and is ignored by the data processing macros. If nonblank, it gives the sampling state that <i>starts</i> at this time that should be used for the instruments connected to the data acquisition system (and associated with “sample line 1”) if the state values computed from the sampling flags are inappropriate. This state is used for this and all subsequent times until a different value is given in the event log. The state numbers must be the same as indicated in the “Sampling State Codes” section, above. The code “x” is used to indicate that all data starting at this time are to be rejected. The code “A” is used to indicate that the default states computed from the flags should be used from this time forward.	C [f]
Description	A description of the event or why the state number is being entered manually.	E
Offline or Non-Standard States for Selected Channels	This is used to manually enter states for specific instruments (or for instruments on “sampling lines” other than “1”) when they are different from the others connected to the DAS system, or to indicate when particular instruments are offline or not outputting valid data. States given here take precedence over those given in the “Event Log”. Note that entries are given for each channel of data provided by the data logger, so if an instrument has more than one channel (e.g., “NO” and “NO <sub>x</sub> ” for a NO <sub>x</sub> analyzer) then separate entries should be given for each channel.	[e]
Channel	Data channel name that uniquely identifies the measurement and instrument used, or the “sampling line” number whose state is to be defined. If the former, it must match the name used in the “Channel Name” column on the “Data Channel Control” sheet, as described below. Sampling lines are identified by the string “Line <i>n</i> ”, where “ <i>n</i> ” refers to the line number, which should be greater than 1. (Manual entry of states for “Line 1” are input using the “Operation and Event Log” section, as indicated above.	C [f]

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Date and Time	Date and time the manually input state begins. All times must be in ascending order for any particular instrument or the data processing macro will abort with an error message. However, it is acceptable for times not to be in order if they refer to different instruments, which means that entries for the same instrument can be given together, if desired.	C [f]
State	Sampling state that should be assigned to this instrument starting at this time and continuing until indicated by a subsequent entry in this field. An “x” is used to indicate the data are not to be used, and an “A” is used to indicate that the states computed from the flags (or given in the event log) can again be used.	C [f]
Comment	A comment indicating why the state is different than the default or why the data are being rejected, as appropriate.	E
<u>“Data File Control” Sheet</u>	Used to indicate which data files are to be used to obtain continuous monitoring data for the run, and the format of the data in those files. Must be appropriately filled in before the data can be loaded. See Table 7 for parameter values that should be used for various types of raw data files that are currently in use.	[g]
Source File Type (“Type”)	The type of source file as indicated on the “Data Source File Type” column in the “Data Channel Control” sheet. This is used to associate this type of file with a particular set of data channels.	A, D
Source File format (“Fmt”)	The format of the data in the file: “tab” = tab separated values, “csv” = comma separated, “xls” = Excel file. Note that if the file is an Excel file, the file should either have only one worksheet or it should have a worksheet called “data” where the data will be read.	A, D
Date Column in File (“Date”)	The column number in the file where the date is given. If blank, the date must be given in the “Date (if not in file)” column.	A, D
Time Column in File (“Time”)	The column in the file where the time of day is given. If it is the same as the “date” column this means that the date and time are given together in the same column.	A, D
Time Units per Day	If the time is given in a separate column with the date and using a non-standard, this column gives the number of time units. “1” means that it is the standard hh:mm format that is loaded into Excel where 1 day = 1.0, while “24” means that it is given as decimal hours, as used for raw TDLAS data files.	A, D

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Header Record Indicator ("Hdr Ind")	The code used to indicate whether an input record had header data. "rec1" means that the first record is always the header record. "none" means that there are no header records and the column for the types of data are indicated in the "Data Source Label or Column" column in the "Data Channel Control" as a column number.	A, D
Data Record Indicator ("Data Ind")	The code used to indicate whether an input record contains the data to be loaded. "none" means that all records (except the perhaps the first) are data records.	A, D
Valid Data Check #1 ("Check 1 Col" and "Check 1 Flg")	Codes used in input records to indicate valid data of this type. The "Col" column gives the column number or code (if column headers are used) for the valid or applicable data flag is located, and the "Flg" column gives the value the flag or data in that column to be equal to for the data to be loaded. Records not matching this flag in this column are ignored. This check not done if the "Col" column is blank. Currently used to test for TDLAS channel corresponding to the desired species.	A, D
Valid Data Check #2	Codes used in input records for a second check that must be passed to indicate valid data of this type. Format same as "Valid Data Check #1" columns. If blank, this second check is not done. Ignored if "Valid Data Check #1" columns are blank. Currently used to test for TDLAS flag corresponding to "sample" mode.	A, D
Network Location	The code used to indicate the network location relative to the computer being used. These codes are associated with network locations in the control parameter file, ChamWork.xls, on the local computer. If this is blank (or the code "local" is used, then the full local or network path name should be given in the "Folder" column in this sheet.	A, D
Folder	The subdirectory or folder where the file is located relative to the standard network location as indicated in the control parameter file, or the full path name for the file if the network location is not given in the previous column.	A, D [g]
File Name	The name of the file. If blank or "-", this row is ignored.	A, D
Date (if not in file)	The date for the data in the file if that information is not given in the file.	A, D [g]
OK?	The data loading macro places an "ok" in this column if the data have been successfully loaded. If the "load data" macro is run again without initialization, the macro does not attempt to re-load the data if an "ok" is in this column. These columns are cleared if the data are re-initialized	H

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
<u>“Data Channel Control” Sheet</u>	Used to describe all continuous monitoring data channels and sampling state flags read from the data files listed in the “Data File Control” sheet, give the information needed to locate the data in those files, and give the parameters needed to properly process the data for these channels. The template should indicate the usual configuration for the current experiments, but this may need to be modified if different instruments are used for a particular run.	[e]
Channel Name	The unique identifier for the channel indicating the species monitored and the instrument. Must be consistent with those given in the Instrumentation Information File, InstInfo.xls. Ignored for sampling state flag channels.	A, D
Chadpro Name	The Chadpro designation for the species or parameter being measured.	B [h]
Chadpro InstID	The Chadpro designation that uniquely identifies the instrument. Must be consistent with that given for the instrument on the InstInfo.xls file.	C, D
Priority (“Pri”)	The Chadpro priority designation for the channel, with “1” indicating highest priority and “3” indicating the data are unreliable.	C, D
Corr Factor	The calibration factor to be used when processing the data for analysis or modeling. The data are processed using $(\text{Processed Data}) = (\text{Factor}) \times [(\text{Raw Data}) - (\text{Zero})]$ This should be manually entered unless it can be computed automatically from the zero and span data.	C, H [I]
Note	Space to put footnote documenting source of factor, if non-default value used. (Autocalibrate macro enters an “A” here)	E
Corr Zero	The zero offset correction to be used when processing the data (see above). This should be manually entered unless it can be computed automatically from the zero data.	C, H [I]
Note	Space to put footnote documenting source of zero correction, if non-default value used. (Autozero macro enters an “A” here.)	E
Time Offset	The difference between the time given with the data in the raw data file and the time the source was actually sampled, in minutes. Should be positive if the time given with the data in the file is later than the time that really should be used with the data.	C, D [x]
Min Data OK Max Data OK	The range of acceptable values for raw data for it to be processed. Data outside this range are rejected. If blank, then no range checking is performed.	C, D [x]

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Data Source File Type	This is used to indicate which type of file contains the data for this channel. It must match a file type given in the first column in the “Data File Control” sheet. If it is blank the data are not loaded and the channel is not used.	A, D
Data Source Label or Column	If the source file for the data has headers, this gives the label used in that file to identify data from this channel. If it does not have headers, this gives the column number that has the data for this channel.	A, D
Sample Line or Flag	<p>For data channels that refer to experimental measurements, this gives the “sample line” that is associated with the source of the data. “Sample line 1” is by definition the main sample line used for the continuous analyzers, and “1” should be given here for all species monitored using this line. “Sample line 0” refers to species that always refer to the same state, or don’t refer to any particular state, as generally is the case for temperature or light intensity measurements, for example. “Sample lines” of “2” or greater can be used for channels that are controlled by their own flags, and the corresponding codes relating these flags to sampling states must be given in the “Sample Inlet Control” sheet.</p> <p>For input channels that refer to flags used to compute sampling state, the input here should be “Fn”, where “n” refers to the flag number. These are used to compute the sampling states as indicted in the “Sample Inlet Control” sheet.</p>	
Residence (“Res”) time	Residence time in the sampling line used. Not currently implemented.	X
Stabilization (“Stab”) time	The number of minutes in the state required before data from this channel can be considered to be valid. Should be at least 3 minutes to allow for equilibration of the sample line when the valves are changed. But may have to be set to a longer time if the instrument takes a long time to respond, as is the case for the Alpha Omega formaldehyde analyzer. Note that if this exceeds the maximum time in the state provided by the sampling schedule, then no data will be processed.	C, D [x]

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Calibration Source State Cal Source Concentration	If automatic calibration is to be used when processing data for this channel, these give the sampling state number that corresponds to sampling span gas for this species, and the concentration of the species in that span sample. For species where this is appropriate, the template gives the sampling state number and calibration concentration as given in the “Cal Sources” sheet, discussed below. This column should be left blank if automatic calibration is not to be used even if there is an entry for this species in the “Cal Sources” sheet. Otherwise, the calculation in the template, which uses the data in the “Cal Sources” sheet value, should be used.	C, G [j]
Use Auto Zero	Enter “yes” if it is desired to automatically compute the zero correction from the zero air sampling data for this channel. Clear this column or enter “no” if the zero correction is to be manually entered, or the default of 0 (no correction) is to be retained regardless of the zero air sampling data.	C, D
“Reject n x Sdev”	The automatic computation of zero and calibration factor corrections are made by averaging the values in the zero and in the applicable span mode. When calculating these averages, the program can optionally reject data more than a given factor times the standard deviation away from the average. If this column has a nonblank number, then data more than that factor times the standard deviation from the average will be rejected. If this is blank or zero, then no data are rejected on this basis. It is NOT recommended that factors less than 3 be entered.	C, D
Zero Avg Zero Sdev Cal Avg Cal Sdev	These are the averages and standard deviations of the zero samples and the applicable span state (if specified in the “Cal Source State” column) that is calculated from the processed data. They are output when the data are calculated. These are used when the Auto Zero Span procedure is executed, and are updated to the new values once the calculated zeros and spans are applied.	H

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Initial or Average Data for Run States of Interest	These columns give the initial or average concentrations for selected states, which may be useful for modeling purposes. An “I” in the “Typ” column means compute the initial concentration at the time the lights are turned on, and an “A” means compute the average concentration for the time the lights are turned on. When computing the initial concentration, the average between the time specified in the “Injections Complete” cell in the “Log” sheet and the “Lights On” time specified in the same sheet is used. If no entry is given in the “Injections Complete” column, then the average is for the half hour before the lights are turned on. When computing the average, the data between the time the lights are turned on and off (or between lights on and the last data point if the lights off time is not specified on the “Log” sheet) is used. The state is specified in the heading, and should be the same as the state’s “Sheet Name” as specified in the “Sampling State Codes” section in the log sheet. These should be the same states for which Chadpro output files are produced, as indicated in the “Chadpro Output File” entry in the “Sampling State Codes” section of the “Log” sheet.	
Type (“Typ”) Value for Specified State(s)		C, D [k] H
Comments	Comments about special problems encountered with this channel, such as when the span or zero correction factors are particularly uncertain.	
<u>“Cal Sources” Sheet</u>	This is used to enter span information that can be used to automatically calculate span factors for species for which span sources are sampled. The template provides for NO and CO spans (as State “4”) and use of Gas Phase Titration (GPT) to provide spans for O <sub>3</sub> and NO <sub>2</sub> (as State “5”). At present, only one span state can be used per compound.	[e]
Compound	Chadpro name of the compound being calibrated. This must match the name given in the “Chadpro Name” column in the “Data Channel Control” sheet for the channels with data for this compound.	C
Span State Number	The state number for when span gas with this compound is being monitored. Must correspond to the state number as given in the “Code” column in the “Sampling State Codes” section of the “Log” sheet.	C, D
Concentration	The concentration (in the desired units for the processed data) of the compound in the span gas. Although the template may have default values for some species, THIS NEEDS TO BE CHECKED and as appropriate updated for each run.	C

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Date Last Checked	The latest date that the given span gas concentration was determined to be appropriate.	E
Other Cal Source Documentation Information	The comment in the template should ALWAYS be replaced by some comment that will indicate that the default value was not used without checking.	E
<u>“GC Data” Sheet</u>	This is used to enter all GC data taken in association with the run. Currently all these data must be entered manually, but eventually macros will be prepared to load these data from the HPCHEM data files. Therefore, the format of this sheet is subject to change.	
Sampled Compound List	This gives a list of at least all the compounds sampled in the run, along with their calibration factors. It may also include compounds that are not sampled in this particular run, which are ignored when the data are processed.	[e]
Compound and Instrument	This gives the computed combination of the compound and instrument that is used to look up the calibration factor in the section where the measured data are entered. These cells contain calculation formulas that should be copied to any new columns that are created.	G [1]
Instrument	The Chadpro identification number or code for the GC instrument	B
Compound	The Chadpro name of the compound being monitored	B
Priority	The priority of the data, where “1” means that the data are most reliable, and “3” mean they are not reliable.	C
Factor	Calibration factor, giving concentration units per unit GC response.	B
Ndat	Number of data points found with this compound and instrument when processing the data, and column number on the processed data sheets. These are output by the data processing macro.	H
Col		H
Initial Concentrations	Initial concentrations (average for time between when injections stabilized and lights on, or for 30 minutes before lights on) for the species for the states of interest. The states are copied from those given in the “Initial and Average Data” headers in the “Data Channel Control” sheet. If additional states are added on the for this purpose on the “Data Channel Control” sheet, then columns should be inserted before the narrow column on the GC sheet and the formula referring to the header should be copied from the previous column.	C, H



Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
GC Data For Run	This section is used to enter the results of the GC measurements made during the experiment. Each instrument and species name combination given here should match an entry in the “Sampled Compound List” section.	[e]
Code	The sampling state number indicating what was sampled, e.g., “0” for pure air, “1” for reactor (or Side A), etc. Must correspond to the state number as given in the “Code” column in the “Sampling State Codes” section of the “Log” sheet.	B
Date and Time	The date and time when the sample was taken	B
Instrument	The Chadpro instrument ID number or code. Must match the instrument ID used in the “Sampled Compound List” section.	B
Compound	The name for the species being sampled. Must match the compound name given in the “Sampled Compound List” section.	B
Area	The peak area or GC response measured for the sample	B
Concentration	The concentration for the sample, calculated using the factor given for the compound and instrument combination in the “Sampled Compound List” section.	B, G [I]
Ok	Used by the macro to indicate that data have been processed	H
Comment	Space available for the operator to enter any comment that may be useful regarding the data point.	
<u>“Sample Inlet Control” Sheet</u>	This sheet is used to determine the sampling states that go with the various sample lines that are associated with the individual continuous monitoring data channels using the “Sample Line” column in the “Data Channel Control” sheet. If the sampling states for a sample line depend on flag values, this sheet gives the sets of flag values that correspond to each state.	
Sampling Setup	A code referring to a physical configuration of the sampling lines and associated valves as employed during the experiment. This should refer to a setup ID given in the “Sampling Setups” sheet of the Valve State Control file (valves.xls), which gives additional information and documentation for this setup.	E
Sampling Setup Format	A code indicating the format of the sampling setup data in the file so the data processing macros can determine how to process it. This should not be modified except as directed by the Data Processing Manager	A, D

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Number of Sample Lines	The number of different sample lines as determined by the data loading procedures.	H
Maximum Flag Number	The number of flag channels as determined by the data loading procedures	H
Number of Operator Logs	Number of sections in “Log” file where operator logs can be input. Currently should always be “1”	A, D
Line State Assignment Section	This section is where the information associating the states to the lines is given. (Note that “line 0” must always be associated with a single state – generally the reactor state – and the columns giving the assignment type and the associated flag values are blacked out for that line.) There should not be any blank rows between or within those giving the line definition input.	[e]
Line	The line number. The first should be for “line 0” but the subsequent line numbers can be in any order. If blank, the input is applicable to the line given above.	A, D
State	The sample input state to be assigned to this line, either always or if the given flag values are matched, depending on the information in the data in the “type” or “input flag values” columns.	A, D
Assignment Type	The type of assignment, which should either be “always” or “match flags”. The “always” type means the given state number is always associated with this line. The “match flags” type means that the state numbers depend on the flag values. In following lines give the state numbers in the “state” column and the flag values corresponding to them in the “input flag values” columns. (This column is not used for Line 0, which is always of the “always” type.)	A, D

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Input Flag Values	<p>The flag identifiers and values used for “match flags” assignments. Not used for Line 0 or “always” type assignments.</p> <p>The first row for the line gives the flag IDs, which must match a name for a flag channel as given in the “Channel Name” column in the “Data Channel Control” sheet. There should not be any blanks in the list of flag IDs until all the flags are specified, since a blank flag ID indicates there are no more flags to examine, and subsequent columns are ignored.</p> <p>The next rows give the flag values that that correspond to the state number given in the “State” column for that row. All flag numbers should match those that are given in this row if the indicated state is to be used. If the state doesn’t depend on the value of a particular flag listed in the first row for the sample line, then the cell for this flag for this state should be left blank. Note that the flags do not necessarily have to be binary, but for binary flags the allowable values are “0”, “1”, or blank for off, on, and “don’t care”, respectively.</p>	A, D [o]
<u>“Model Input” Sheet</u>	<p>This sheet is used to assign or derive input data for modeling this experiment and is generally maintained by the run modeler. Macros can be accessed from this sheet to produce model input files or model evaluation data files that can be used by the model programs. No information on this sheet is used by the data processing procedures, but references are made to data processing results where appropriate. Defaults are appropriate for current experiments, and the template should be updated when the conditions of the current experiments change.</p>	
Run ID	Copy of the run ID from the log sheet	G
Characterization Set	Name of the data file used to give the characterization information for the conditions of this experiment.	D [m]
k1 (min <sup>-1</sup> )	NO <sub>2</sub> photolysis rate assigned to the experiment.	D [m]
HV	Set to 1 if a lights on time is given, indicating that this is a photolysis experiment.	G
Spectral Distribution	The spectral distribution file assigned to the run. Use of spectral data taken during the experiment for computing a run-specific spectral distribution has not been implemented.	
Run Time (min)	The irradiation time computed from the lights on and the lights off times given in the Log sheet.	G

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Model Output Time	The frequency for outputting calculation results, in minutes. Appropriate value depends on duration of experiment and how rapidly concentrations are changing.	
Side Specific Assignments	Assignments for the specific reactors or sampling states being modeled.	
State Designation	The designations for the sampling state for the reactor being modeled. Must match an appropriate "Sheet Name" given in the "Sampling State Codes" section of the "Log" sheet.	D
Side Designation	The designation used in model input files for the experiment in this reactor. Template uses entry given in the "Chadpro Output File" column in the "Sampling State Codes" section of the "Log" file.	G
Temperature	The average temperature to use when modeling the run. Template uses average temperature computed for the temperature channel on the "Data Channel Control" sheet.	G
Dilution	Dilution rate to be used when modeling the run, if not zero. Default is blank for no dilution.	D [m]
OK to Model?	A "yes" in this column means the macros invoked from this sheet will output a file for this reactor.	D
Initial Concentrations	This section is used to input initial reactant concentrations that must be specified when modeling this run. This is split into three sections: (1) initial concentrations from continuous monitoring instruments that can be derived from the calculated initial concentration data on the "Data Channel Control" sheet, (2) assigned initial concentrations for unmeasured species that must be manually entered, and (3) initial concentrations derived from data in the GC data sheets.	[e]
Model Name	The name of the species that is used for modeling. Usually this is the same as the Chadpro name.	D [n]
Channel Name or GC species	For continuously monitored species, this channel name used in the first column of the "Data Channel Control" sheet that corresponds to the measurement to be used to derive the initial concentration of the species. (If the species is measured by more than one instrument, this is the measurement from the instrument considered to be the most reliable). For GC species this is the GC instrument ID that should be used as providing the most reliable measurement for this species. This must match the GC instrument IDs used on the "GC Data" sheet. This column is ignored for assigned species.	D [n]

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
Units	The concentration units of <i>the processed data</i> . If “ppb” the processed data value are divided by 1000 when producing model input files.	D
Reactor concentrations	The computed or assigned concentrations for modeling. For the computed values given for continuous or GC species, the calculation formula from the appropriate section should be copied to any new rows of this type if such have to be created to input additional species.	G
Model Input Files	This is the model input file computed from the input data given in the previous sections. It does not need to be modified by the user unless it is necessary to insert rows in the “initial concentrations” section. If rows are inserted there, then the corresponding rows need to be inserted here, and the formulas copied as instructed on comments in the sheet.	G
<u>“Loaded Data” Sheet</u>	This sheet is used to store the unprocessed data and flags loaded from the input files for the continuous instruments. All data on this sheet is produced by the “load data” macro, and the sheet is erased whenever the data are initialized. No user input or edits should be made on this sheet.	
Time	The date and time array produced when the data are initialize, based on the data start and end times and the data time interval given on the log sheet. The first time is the data start time, and the subsequent times are incremented by the time interval until the data end time is reached. The loaded data are then aligned with these times, and then offset by the number of rows based on the data in the “Time Offset” column in the “Data Channel Control” sheet.	H
“Op Log 1”	The log codes from the “Event Log” section of the “Log” sheet are inserted here in the appropriate time slot.	H
“Line <i>n</i> ”, where “ <i>n</i> ” refers to a sample line number.	The sampling state codes for the various sample lines as computed from the state flag values are stored here.	H
Species Data (two columns per data channel input) Or Flag Data (one column per flag channel input)	The header gives the “Channel Name” as given in the first column in the “Data Channel Control” sheet. For species data, the first column contains the raw species concentration for the time as read for that channel from the input file, and the second column contains flags given for the channel in the “Non-Standard States for Selected Channels” section of the “Log” sheet. For flag channels, the flag value is given in the single column used.	H

Table 6 (continued)

Sheet and Designation	Purpose	Notes [a]
<u>Processed Data Sheets</u>	For each sampling state for which valid data are found when the data are processed, there is a processed data sheet containing the processed data for the sample. If no sheet exists for a given defined sampling state with data than one is created. The data in these sheets include GC data as well as data from the continuous monitoring instruments. Each processed data channel has three columns as indicated below. The column for which the processed data occur are the same on each sheet, regardless of whether the sheet has data for all the channels input. A set of columns are allocated for each continuous channel for which non-blank input is given for the data source file type and column, regardless of whether data of this type were found or not. After these, columns are allocated for each GC channel in the order given in the “Sampled Compound List” section of the “GC data” sheet. A set of columns are allocated for each GC channel on that list regardless of whether run data are input for that channel or not.	
Time	The clock time for the measurement. Only times with valid processed data for this channel and sampling state are given; times with invalid or rejected data or data associated with other sampling states are not included.	H
Min	The minutes after lights on or after the data start time if lights on time is not given	H
Channel Identifiers and Data	<p>The first row gives the channel name, which is the given in the “Channel Name” column on the “Channel Data Control” sheet for continuous data or the “<i>species name; instrument ID</i>” for GC data.</p> <p>The second through fourth rows give the Chadpro name for the species measured, the identifying code for the instrument used, and the priority number, as given in the “Data Channel Control” sheet for continuous channels or the “Sample Compound List” section of the “GC data” sheet for GC data.</p> <p>The remainder of the rows give the processed measured data, with appropriate calibration factors and zero corrections and time offsets applied.</p>	

[a] Codes for notes are as follows:

- A Must be entered before data can be loaded and plotted
- B Must be entered before data can be processed .
- C Data can be processed without providing this information, but the results may not be suitable for modeling
- D The default value should usually be used. The template should be updated if the default value is no longer appropriate for the current experiments.

Table 6 (continued)

- E Not needed for data processing but should usually be provided for documentation
  - F Not generally provided except as directed by the project scientist
  - G Calculated data. Do not modify.
  - H Filled in by macro.
  - X Presently unused but reserved for future use.
- [b] This should be updated appropriately in the run template whenever daylight time begins or ends.
- [c] Data can be processed without providing this information, but the results may not be suitable for modeling.
- [d] The current template should have the appropriate designations for the number of reactors used usually. If not, the template should be modified accordingly. A consistent system should be used when designating reactor letters, so the Project Scientist should be consulted if it is not obvious how to assign the reactor designation letters.
- [e] Add this information only in the space provided in the template, not in rows indicated by gray or in rows below that. If it is necessary to add more comments or entries than provided by the template, then insert the needed rows above the gray area. This is necessary for the data processing macros to process all the rows with this information. Blank rows are permitted and are ignored by the data processing macros.
- [f] Required before automatic zero or span corrections can be made if the flag values do not correctly indicate the zero and span modes.
- [g] The template will calculate names and locations for the default input files given the data start and end times given for the log sheet for runs of up to five days. These calculated file names and locations will need to be manually modified if non-standard names and locations are used. The color should be changed from blue to red if manually modified.
- [h] Required for using the automatic zero or span macros.
- [i] The “automatic calibration and zero” macro will over-write this with the calculated value and change the color from red to purple to indicate that it was produced by a macro.
- [j] Clear these cells if automatic calibration is not to be used for this channel. If these columns are blank and it is desired to use automatic calibration for this channel, the calculation cells in rows where it is nonblank should be copied into the row for this channel. DO NOT manually enter calibration state numbers and concentrations here, since the calibration information should only be entered, these should only be entered in the “Cal Sources” sheet.
- [k] The template provides for two states for which the initial or average concentrations will be computed. If it is desired to have this computed for additional states, then columns can be inserted before the narrow column at the end, and the desired state’s “Sheet Name” can be entered in the header.
- [l] If new rows have to be added, then the formulas used should be copied into this location from another row of the same type
- [m] The default can be used for initial assessment purposes if the experiment represents the conditions reflected in the template, but these may need to be refined before the run is finalized.
- [n] Most of the species in the template default probably should be kept, but it may be appropriate to add additional species.
- [o] If more flags need to be added than provided for in the space them in the template, then new columns can be added to the left of the gray column.
- [x] The default values given in the current template should be checked for appropriateness and revised as needed.

Table 7. Parameter values that should be specified in the run data files when reading data from the various types of raw data files that currently can be processed.

File Type	Parameter in “Data File Control” sheet [a]							How Data Specified in the “Data Channel Control” sheet [b]
	Fmt	Date Col	Time Col	Units /day	Hdr Ind	Data Ind	Date [c]	
Primary DAS Raw Data Files (“1M”) files	csv	2	3		HDR	DAT	N/A	Give label that matches header label [d]
Valve State Files	tab	2	2	1	none	none	N/A	Column Number (starting at 4)
Raw Serial Data from TDLAS	csv		1	24	none	none	yes	Concentrations in column 3; correlations in column 4. See note [e]
Raw Data from TDLAS #1 (NO <sub>2</sub> and HNO <sub>3</sub> data)	tab		1	24	none	none	yes	Data column labeled “mr”
Raw Data from TDLAS #2	tab		1	24	rec1	none	yes	Data in column 4
Recommended Format for Processed Data Files	xls	1	1		rec1	none	N/A	See note [f]

- [a] See description of the “Data File Control” sheet in Table 6 for a description of these parameters.
- [b] This refers to the header label or column number given in the “Data Source Label or Column” column.
- [c] “yes” means that date is not in the file and it must be specified in the “Data File Control” sheet and “N/A” means that the date is given in the file so it need not be specified externally.
- [d] The header labels used for each species/instrument combination processed using the DAS system should be given in the “DAS Connections” sheet of InstInfo.XLS.
- [e] Data for both channels are included in this file, with column 2 giving the measurement type, where 0 and 1 corresponds to NO<sub>2</sub> and HNO<sub>3</sub>, respectively, for TDLAS#1 and 0 and 1 corresponds to H<sub>2</sub>O<sub>2</sub> and HCHO, respectively, for TDLAS#2. The measurement mode is in column 5, and only data with measurement mode of “3”, indicating “ambient sample”, should be loaded. See discussion of “Valid Data Check(s)” in Table 6.
- [f] The recommended format for processed data files is for the data to be read into the data processing program to be in a sheet named “data”, where the first row has the header information and the first column has the time and data in Excel time/date format. The data column should have the appropriate label, which is matched by the label given in the “Data Source Label” column in the “Data Channel Control” sheet. Columns of other information should also be given, if desired, but there should be no blank column headers in any columns before the column for the data to be loaded.



Table 8. Description of controls and macros that can be used to load and process data in Run Data and Current Data files

Procedure Label	Description
Data Loading Procedures	
Initialize	<p>Erases all data in the “Loaded Data” sheet (i.e., all data for channels listed in the “Data Channel Control” sheet), if any, and creates a new time array in the “Loaded Data” sheet. The Data Start Time, Data End Time, and Time Interval must be defined on the “Log” sheet before this can be run. This must be run before the “Load Data” macro is run.</p>
Load Data	<p>Loads the data for the channels listed in the “Data Channel Control” sheet from the files listed in the “Data File Control” sheet, using the file names, parameters, and associations given on these sheets.</p> <p>The “data source” parameters in the “Data Channel Control” and the file names in the “Data File Control” sheet must be appropriate for this run. The “Initialize” macro must be run first.</p> <p>Once a file is loaded, an “ok” appears next to it on the “Data File Control” sheet. If “Load Data” is run again without re-running “Initialize”, only the files with out an “ok” will be loaded. Therefore, if a file wasn’t loaded because it had an incorrect name or parameters specified, “Load Data” can be run again after this is corrected to load only the data from this file, without re-loading the other data. Note that if a file had data added to it since “Load Data” was successfully run previously, it is necessary either to re-run “Initialize” to force re-loading all data, or to clear the “ok” next to the relevant file name when re-running “Load Data”.</p>
Data Processing Procedures	
Process Data	<p>This applies corrections and determines appropriate sampling state for all loaded DAS data and also for GC data (if any) and places the processed data in the various processed data sheets, which are named according to the sheet names given in the Sampling State Codes section of the “Log” sheet. The processed data are then copied to the plot file so the processed data can be viewed in the plots there. Average concentrations in the zero and span states and initial concentrations in the reactor state(s) are also calculated for those channels where this is applicable in the “Data Channel Control” sheet.</p> <p>A minimum requirement for this to run is for the DAS data to be loaded using the “Load Data” macro, and this should allow viewing of plots of the data. However, for the data to be processed correctly the “Data Channel Control” sheet should have the appropriate values for the factors, zeros, offsets, and stabilization times, and any needed manual state specifications or bad data flags must be entered where appropriate on the “Log” sheet. If any of the flags are edited the “Update Flags” macro should be run before “Process Data”, or the “Update Flags and Process Data” control should be used instead. If GC data are present they will be processed as well.</p>

Table 8 (continued)

Procedure Label	Description
Update Flags	<p>This must be run before “Process Data” is run if any state flags are modified by entering manual state codes or flags in the “Event Log” or the “Offline or Non-Standard States” section of the “Log” sheet, or if any stabilization time parameters are changed. It is not necessary to run this after new data are loaded using the “Load Data” command because the flags are automatically updated after new data are loaded using this procedure.</p>
Update Flags and Load Data	<p>This is the same as first running “Update Flags” then running “Load Data”. This can be run after editing or adding state flag parameters or “Log” entries if it is desired to process the data immediately afterwards.</p>
Process GC Data	<p>This control is accessible on the “GC data” sheet and is used to process only the GC data when the DAS data have already been processed. The GC data are copied to the processed sheets for the applicable sampling states, with GC data columns immediately following the columns used for the DAS channels. Initial concentrations of GC species are also computed and entered in the “Sampled Compound List” section in the “GC data” sheet, and successfully processed run GC data are indicated with an “ok” in the row giving the data. It is generally used for data processing after entering or editing only GC data because it takes much less time to run than “Process Data”</p> <p>At least “Initialize” must be run before “Process GC data” can be run.</p> <p>It is not necessary to run this separately after “Process Data” is run, because GC data processing (if needed) is done as part of this procedure.</p>
Auto Zero Span	<p>This is used to compute the zero and span factors (the numbers in the “Corr Zero” and “Corr Factor” columns in the “Data Channel Control” sheet) to give best fits to the data in the zero and appropriate span state for the species. This is done for all species where this option is selected using the “Use Auto Zero” and/or “Cal Source State” and “Cal Source Conc” columns on that sheet, if there are processed data in the zero and/or appropriate span state. If new span and zero factors are calculated, the factors are put in the “Corr Zero” or “Corr Factor” column in purple font, and the “Process Data” procedure is re-run to re-calculate all the data with the new factors, and update the plots on the plot sheet.</p> <p>At a minimum “Process Data” must be run first, and the appropriate parameters must be specified in the “Data Channel Control” sheet concerning which channels to use and giving their appropriate span state and concentration. However, for the results to be correctly calculated, the correct span concentrations should be entered in the “Cal Sources” sheet, and bad or inappropriate points should be removed using appropriate flag or manual state entries in the “Log” sheet. This is most conveniently done by looking at plots of the data for the relevant channels and states to determine if they all reflect valid and stable readings in the appropriate mode, and if necessary flagging or changing state codes for time periods where the data are inappropriate.</p> <p>Note that points that are more than a certain number (usually three) of standard deviations of the average are not counted when computing the averages that are used for computing auto zeros or spans. Therefore, a few clearly anomalous points may not affect the results. This is controlled using the “Reject n x Sdev” column in the “Data Channel Control” sheet.</p>

Table 8 (continued)

Procedure Label	Description
Compute Avgs	<p>This re-calculates the average or initial concentrations for the DAS channels on the “Data Channel Control” sheet. This is not normally needed because it is automatically run every time “Process Data” is run. It is really only needed if the channels selected for averaging or initial concentrations are changed, and one wants to see the results without re-running the rather time-consuming “Process Data” routine.</p> <p>“Process Data” must be run before this can be run. It may be necessary to add or edit manual state flags on the “Log” sheets to remove inappropriate points for correct average initial concentrations</p>
<p>Window Changing Procedures</p>	
View Plots	<p>This is used to change the active workbook to the data plotting file so the plots of the processed data can be seen. If the data from this run file have not been loaded previously, they are loaded first. Otherwise, it is the same as selecting “EPAplot.xls” using the Excel “Window” menu.</p>
<p>Procedures for the “Current Data” file</p>	
Load and Process Data, then View Plots	<p>This combines the operations of “Initialize”, “Load Data”, “Process Data” and “View Plots” in one macro. The control for it is in the “Data File Control” sheet of the Current Data file, which is normally the only sheet one may need to modify when viewing current data. This is used when first using the current data file, when changing the date or number of days for data to be viewed, or when updating the data when viewing data for the current day.</p>
<p>Model Input Preparation Procedures</p>	
Create INP files	<p>This creates a model input (.INP) file for each reactor state of interest for modeling this experiment. The files are named according to the name given in the “Side Designation” line in the column for each reactor or side of interest, and their locations are as specified by the “ChadINPloc” parameter in the control parameter file.</p> <p>This should normally be run only after all the data are processed sufficiently that the correct initial concentrations are specified, and other model input parameters are appropriately specified in the “Model Input” sheet.</p>
Create GDT files	<p>This creates a run data file in the “general” (.GDT) format containing the concentration-time profiles for the processed data for each reactor or side of interest, using same name as used for the INP files. The file locations are as specified by the “ChadDatLoc” parameter in the “Model Input” file. These files are useful when using some pre-existing modeling programs when evaluating model simulations of the experiments.</p> <p>This should normally be run only after the data are processed sufficiently that they are considered sufficiently well quality-assured for use in modeling. Inappropriate data assigned to the reactor states should be removed, and the best available calibration and zero corrections should have been entered (or computed) in the “Data Channel Control” and “GC Data” sheets.</p>