SPGAS

Reprocessing Tool V 3.1 (Draft)

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CIC Photonics

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Introduction

The SPGAS software is a multi-component gas analysis program comprised of several different tools that allow a user to conduct a complete examination of their gases. Within the SPGAS software package the user is given the means to collect data, calibrate that data, quantify the calibrated data, and adjust and recalculate the calibrated data. All of these options are performed by a different software tool within the SPGAS package.

The tool described in this manual is the quantification reprocessing tool. This tool is a supplemental software program for QMax a program produced to create and adjust the SPGAS required quantification sets.

This reprocessing tool gives the user an opportunity to change the ideal gas parameters and then recalculate the previously established calibration. After recalculating the calibration, the user is provided with a new calibration based on the amended parameters.

Key Features

Within the quantification reprocessing tool there are several important components. These components are as follows:

- Ability to recalculate the concentration of the species
- Opportunity to alter the pressure and the temperature used to calculate the concentrations
- Preference on how to view the results, whether it be a table or a chart
- Capability to easily copy the table format and paste into excel
- User Friendly

System Requirements

Any PC currently available has enough power to execute any of the programs that make the SPGAS software package. At a bare minimum the following requirements must be meet:

- Intel or AMD processor, 166 Mhz
- Operating system of Windows 98, Windows Me, Windows NT 4.0, or Windows 2000
- Memory capacity of 64MB
- Disk free space of 20MB
- Screen resolution of 800x600 w 256 colors

Opening the Quantification Reprocessing Tool

The quantification reprocessing tool can be found in the tools section of the IRGAS folder. To reach the IRGAS folder go to the start menu and programs. At the time there should be a folder labeled IRGAS. Within this folder is the tool section and among the tools is the reprocessing program.

To run the reprocessing tool click on its icon. After a few moments the program should automatically appear. At this point the program is ready to be used. This can be seen below in Figure 1.

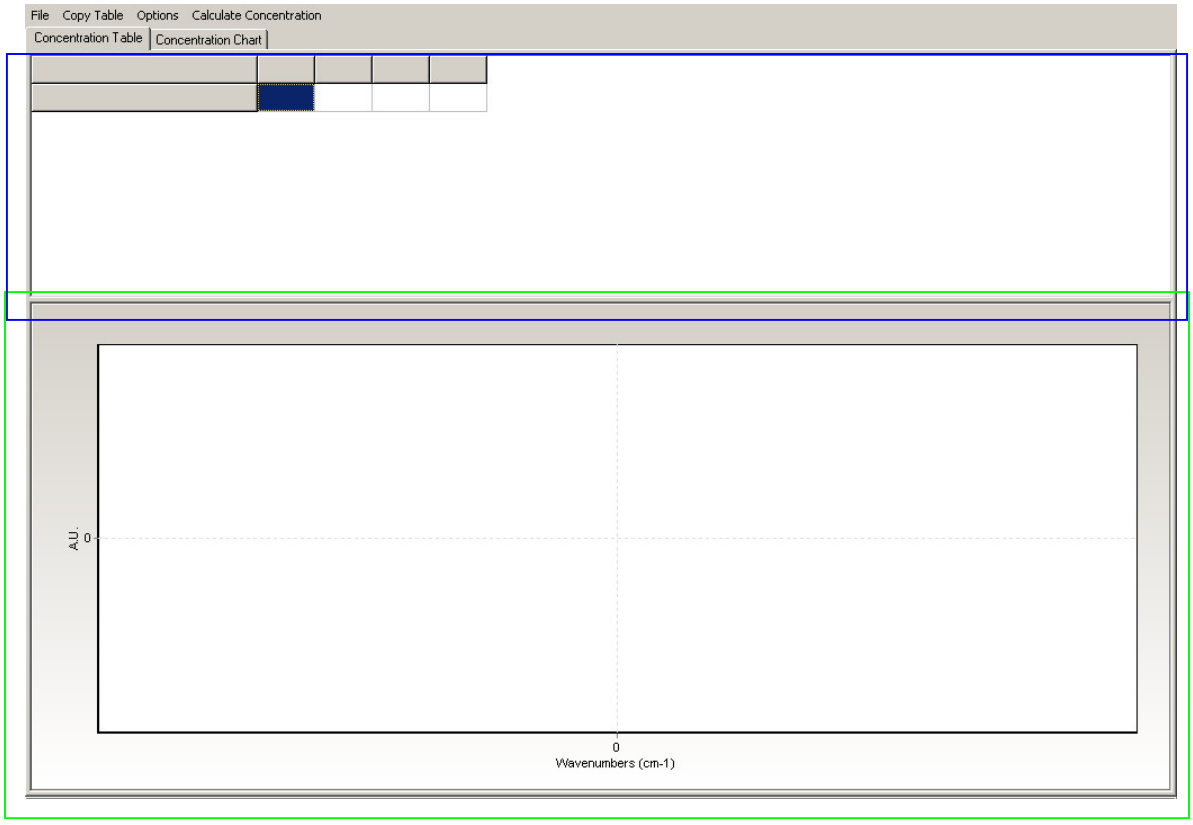

Figure 1 Opening Screen to Quantification Reprocessing Tool

In this starting screen there are several areas you will see. The top portion of the screen is where the new concentrations will be. On the bottom of the screen is the area where the absorbance plot is to be shown. Also at the top part of the screen you will see two tabs, one labeled concentration table and one labeled concentration chart. These two tabs simply give the user the option to choose how the results are presented.

Lastly, the user will see a row of possible drop down menus. Each of these drop down menus provides a different function. All of the areas shown on the start-up screen will be covered in more detail later on in the manual.

Quantification Reprocessing Tool Operation

This section of the manual will cover how to set-up in terms of entering the calibration set and absorbance spectra being used to adjust the concentrations of the species.

Calibration Set

In order to recalculate the concentrations the user must open the calibration set that is to be modified. To do so click on the file tab at the top of the screen . This will bring up drop down menu with options to open a calibration, open absorbance spectra, save results, print or exit. Choose the open a calibration option by clicking on it, as is shown in Figure 2.

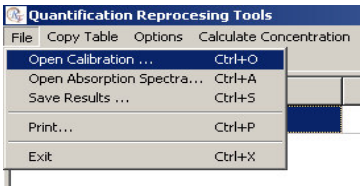

Figure 2 Opening Calibration Set

This will cause another window to appear, in which the user browses for the calibration set from the calibrated spectral database in the IRGAS folder. After the file has been located, click on open. Doing so will place the calibration set at the top of the screen. The user should see their calibration set with its corresponding standard errors in a row at the top of the screen similarly to that, that can be seen in Figure 3.

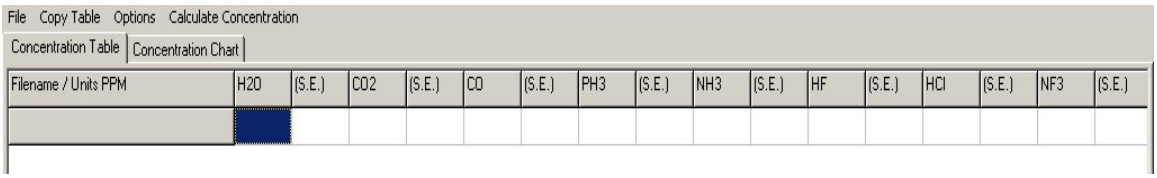

Figure 3 Calibration Set and Standard Errors

Absorbance Spectra

Once the calibration set is in place, the user needs to open an absorbance spectra. The absorbance spectra chosen should reflect the 30 min time span that corresponds to the time period that needs to be adjusted. To open an absorbance spectra click on the file drop down menu again, but this time select open absorbance spectra, as is shown in figure 4.

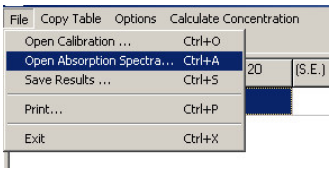

Figure 4 Attaining the Absorbance Spectra

Much like the calibration set, this will pop-up a window where the user will browse for an absorbance spectra that has been collected. This file should be located in a spectral records folder within the IRGAS data folder. Once the desired file has been found, click on ok.

By clicking on ok the absorbance information should now be present on the left hand side of the new calibration area. Refer to figure 5. To see all of the absorbance spectra placed in the program, simply use the scroll bar on the right side of the screen and scroll down.

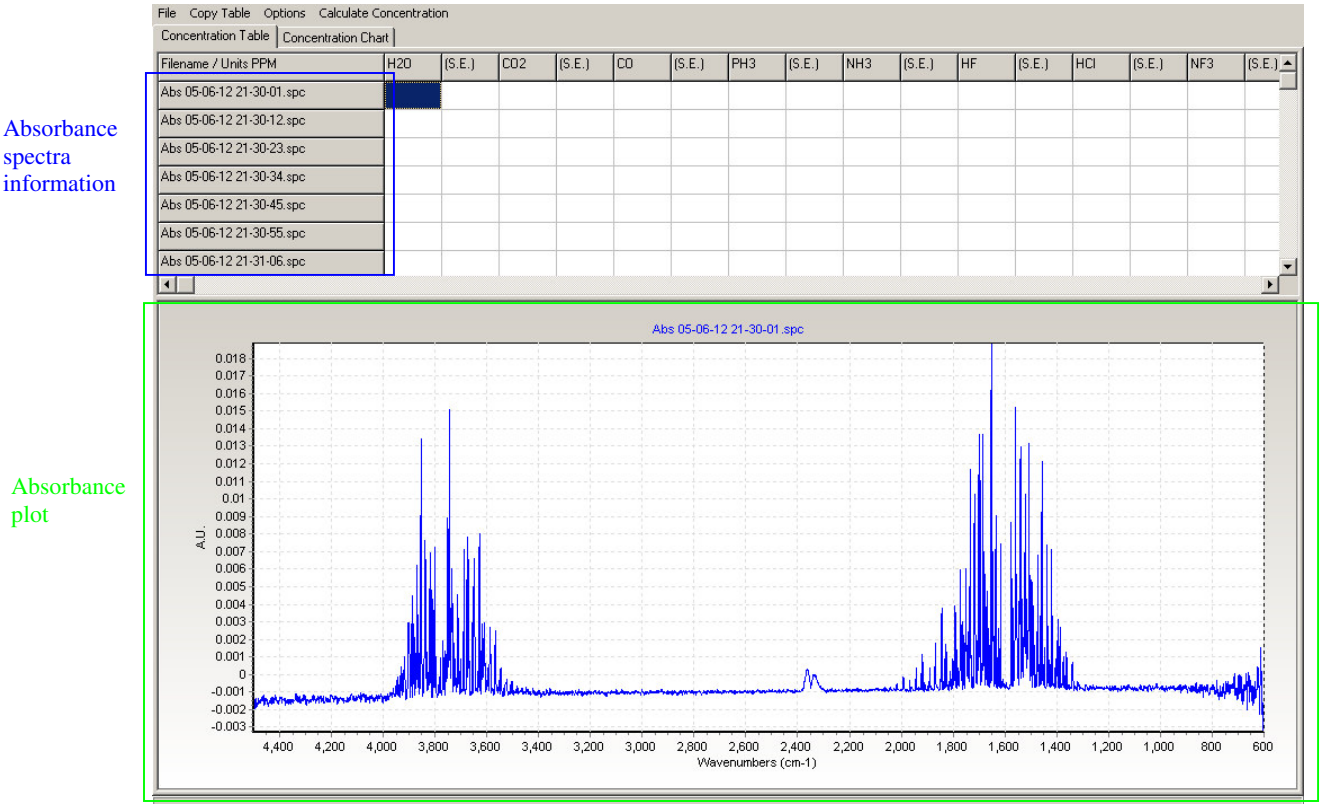

Figure 5 Screen Display of the Absorbance

Also the absorbance spectra should appear at the bottom of the screen as an absorbance plot, as can also be seen in figure 5. In order to see the absorbance plot change with time in respect to the correlating time in the absorbance spectra, click on one of the boxes located within the table and use the keyboard arrow keys to navigate. This action should respond with different plots in the absorbance plot area.

Performing the Recalculation

Covered is this part of the manual will be the steps to take in order to perform the actual recalculation of the concentrations.

Setting the Temperature and Pressure Parameters

Since the entire purpose of the reprocessing tool is to have the ability to change ideal gas parameters and reevaluate the concentration results, the user needs to modify the temperature and pressure used in the calculation before attempting to recalculate. This can be done by referring to the options tab at the top of the screen. Under the options tab are a few selections to choose from. They read pressure and temperature correction, set pressure and temperature, and show residual.

First the user will need to determine what the new pressure and temperature need to be. After that has been decided, click on the options tab causing the drop down menu to emerge. From this menu choose the set pressure and temperature option, see figure 6. This will produce a window . In this window there are areas to enter the pressure and the temperature, refer to figure 7. Enter in the determined values and click ok.

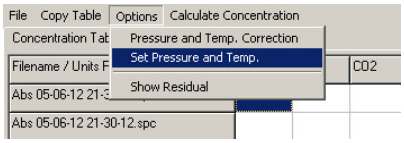

Figure 6 Set Pressure and Temperature Option

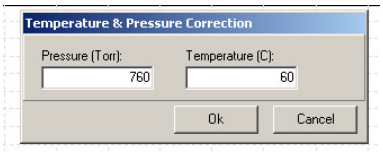

Figure 7 Entering Pressure and Temperature

After entering the pressure and temperature, go back to the options tab and opt for the pressure and temperature correction (figure 8). Following that the options tab is selected again the user should see a check mark next to the option.. This indicates that when the concentration is recalculated it will use the new information in the calculations.

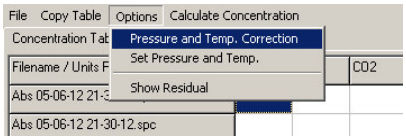

Figure 8 Pressure and Temperature Correction

Calculating the Concentrations

Subsequently, after executing the above actions, the user can have the program recalculate the concentrations. At this time to facilitate this process the user simply needs to click on the calculate concentrations tab at the top of the screen. By doing this the user is having the software recalculate all of

the species concentrations and their corresponding standard errors. Once the program is done the values for the new concentrations will appear in the boxes below the calibration set and to the right of the absorbance spectra. This can be seen below in figure 9.

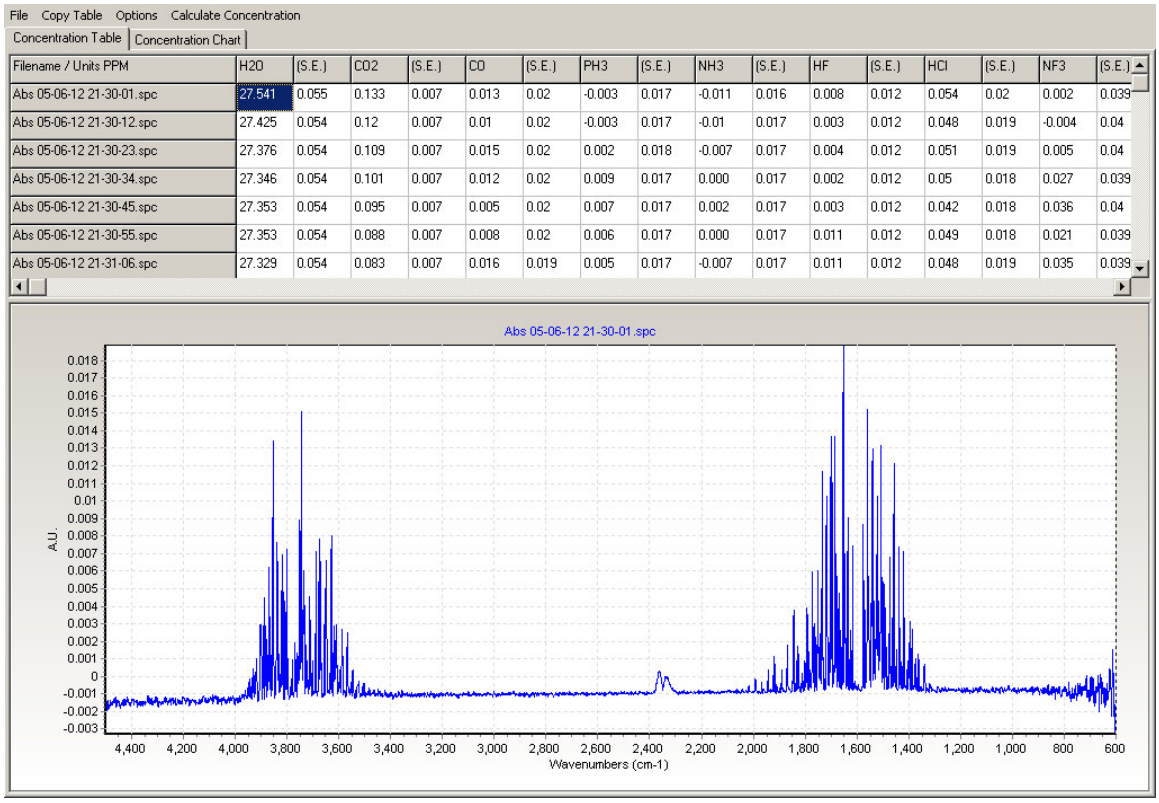

Figure 9 Recalculated Concentrations

User Options

In the quantification reprocessing tool program the user has a few aesthetic options. Some of these choices include being able to copy the concentration table, so as to place in excel, viewing the results as a chart instead of a table, and having the capability to show the residual or not.

Copy Table Option

With this tab the user is given the ability to copy the concentration table by merely clicking on that button. After having the program copy the table, the user can manually open excel and paste the table. The reason this was included in the program is because…….

Concentration Chart Tab

The results of the redone concentrations can be given in two forms. One form is a concentration table which is what is seen when opening the program, the other form is a concentration chart. The user can see the results in the concentration chart by clicking on the concentration chart tab located at the top of the

screen. This action will change screens and the user will now see what is shown in figure 10. This view will look very close to the monitor screen in the IRGAS 100 program.

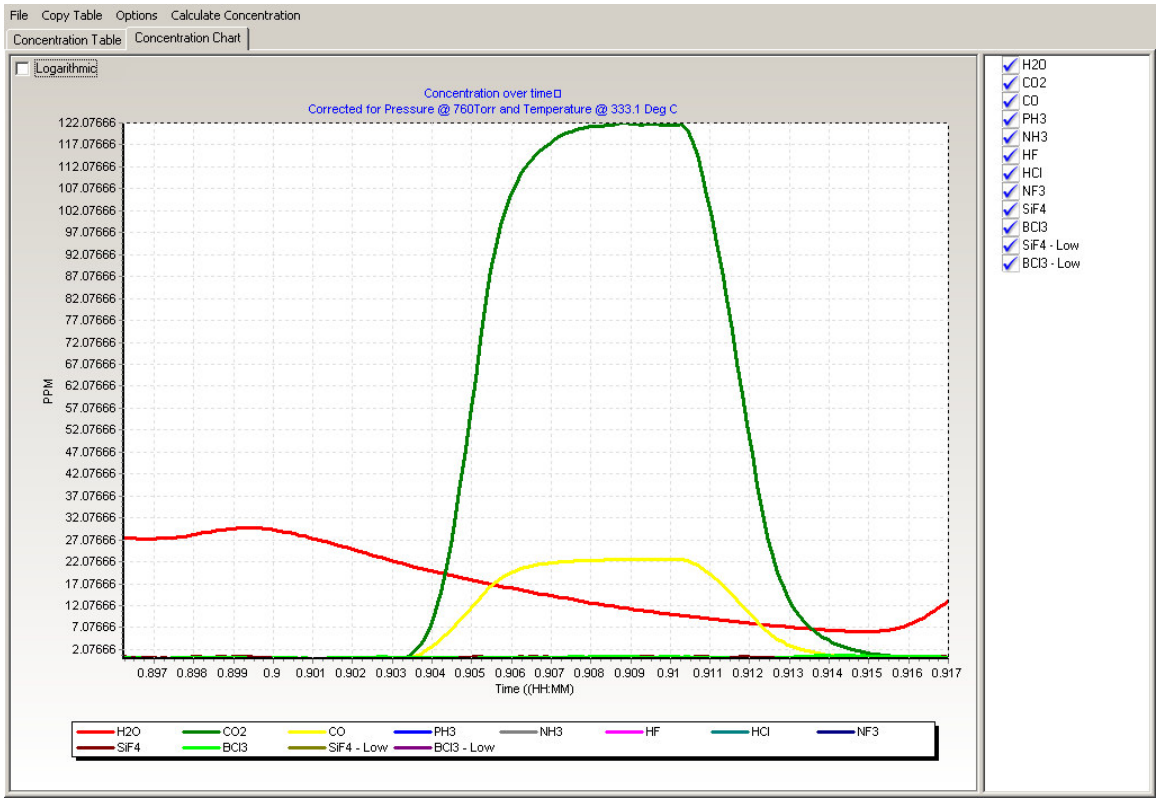

Figure 10 Concentration Chart

Much like the IRGAS 100, in figure 10 there is the species along the bottom (with the choice of which ones to see on the right side), and the plot with ppm vs. time in the center. If the user desires to watch the concentration chart while the program recalculates, then choose this option prior to pushing the calculate concentration button. When the user does this the user can see the concentration chart change over the time being recalculated.

Show Residual

Under the menu from the options button there is a selection called show residual. This choice……..