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GCSOLAR

GCSOLAR.NET User's Manual

Calculating Photolysis Rate Constants of Contaminants in Water

Version 1.0

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U.S. Environmental Protection Agency
Office of Research and Development
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1.0 Introduction

The GCSolar.NET computer application contains a set of routines that computes direct photolysis rate constants and half-lives of chemical and biological contaminants in the aquatic environment. The half-lives are calculated as a function of season, latitude, time-of-day, depth in water bodies, and atmospheric ozone layer thickness.

A graphical user interface (GUI) was developed to facilitate data entry by the user and to make the application interactive. Inputs to the GUI are made via controls such as text boxes, check boxes, drop-down menus, radio buttons, and buttons.

In the case of chemical contaminants, the rates of direct photolysis are computed using simulated solar irradiance values expressed in photon-based units and contaminant quantum yields that are assumed to be wavelength-independent. The contaminants have well-defined UV-visible absorption spectra that are used to compute rate constants for light absorption. A discussion of the chemistry associated with this chemical contaminant application can be found in the following publication:

> "Rates of Direct Photolysis in Aquatic Environment," R.G. Zepp and D.M. Cline, Environmental Science and Technology, 11(4), pp. 359–366 (1977)

This approach used for chemical contaminants has been used to compute photoinactivation rate constants of biological contaminants such as viruses and bacteria. However, the authors found that quantum yields for the viruses were wavelength dependent and decreased with increasing wavelength. Algorithms had to be developed to describe the apparent spectral dependence. However, this approach, although experimentally time-consuming, possibly can be used to obtain a first approximation of calculated rates for biological contaminants.

> "A Modeling Approach to Estimate the Solar Disinfection of Viral Indicator Organisms in Waste Stabilization Ponds and Surface Waters," T. Kohn, M. J. Mattle, M. Minella and D. Vione, Water Research, 88, pp. 912–922 (2016)

An earlier paper, which provided detailed approaches for computing the depth dependence for photoreaction rate constants, introduced approaches for calculating photolysis rates of substances that are complex mixtures of natural organic matter (NOM).

> "Determination of Apparent Quantum Yield Spectra for the Formation of Biologically Labile Photoproducts," W.L. Miller, M. Moran, W.M. Sheldon, R.G. Zepp, and S. Opsahl, Limnology and Oceanography,47(2), pp. 343–352 (2002)

The NOM is made up of mixtures of light-absorbing chromophores and consequently quantum yields of photoproducts are wavelength-dependent. Calculations of the photoreaction rates of these complex mixtures take into account wavelength dependent changes in the solar irradiance that are calculated using the GCSolar.NET software but also consider wavelength-dependent changes in the quantum yields. As data from Kohn et al. (2016) and other results have indicated, similar approaches that account for wavelength dependence of quantum yields are required for computing photoinactivation rate constants of biological contaminants. This early work by Miller et al. (2002) defined a fruitful approach to estimating the wavelength dependence of inactivation of biological contaminants. This approach was further developed in a recent paper:

> "Biological weighting functions for evaluating the role of sunlight-induced inactivation of coliphages at selected beaches and nearby tributaries of the Great Lakes", R. G. Zepp, M. Molina, K.Wong, O.Georgacopoulos, B. Acrey, M. Cyterski, G. Whelan, R. Parmar. *Under internal review.*

This approach defines empirically derived biological weighting functions (BWFs) that quantify wavelength effects on direct photoinactivation of coliphages. Plots of BWFs versus wavelength are referred to as "action spectra." The BWFs are inputs to the GCSolar.NET model in a similar fashion to inputs of molar absorption coefficients for the chemical contaminant modeling. This approach has also been recently used to compute sunlight photoinactivation rate constants of the fecal bacterial indicators, *E. coli* and enterococci:

> "Modeling the Endogenous Sunlight Inactivation Rates of Laboratory Strain and Wastewater *E. coli* and Enterococci Using Biological Weighting Functions," A.I. Silverman, K.L. Nelson, Environmental Science and Technology, 50(22), pp. 12292–12301 (2016)

The users of GCSolar.NET should be aware that the equations used to compute the irradiance at the Earth's surface are most appropriate for terrestrial systems compared to marine systems. For example, Baker et al. (1980) discuss key differences in parameters used in GCSolar.NET and models used to accurately compute solar spectral irradiance at the surface of the equatorial Pacific.

> "Middle Ultraviolet Radiation Reaching the Ocean Surface," K.S. Baker, R.C. Smith, and A.E.S. Green. Photochemistry and Photobiology, 32, 367–374 (1980).

Also, GCSolar.NET uses data for the absorption solar ultraviolet radiation by pure water that are derived from studies of the "clearest natural waters" at the time the program was developed. Since then, newer results have shown that solar ultraviolet radiation penetrates much deeper than estimated by GCSolar.NET.

> "Optical Properties of the "Clearest" Natural Waters," A. Morel, B. Gentili, H. Claustre, M. Babin, A. Bricaud, J. Ras, and F. Tieche .Limnology and oceanograph*y*, *52*(1), 217–229 (2007).

Chapter 2 provides an introduction to each component of GCSolar.NET, and Chapter 3 provides a walkthrough of using GCSolar.NET for a specific chemical scenario.

GCSolar.NET will need a computer running Microsoft Windows 10 with a .NET framework version of 4.0.30319 or newer. It needs a minimum storage of 2.6 MB and a minimum RAM of approximately 25 MB in addition to the operating system's RAM requirements.

2.0 User Guide by Module

The GCSolar.NET program will launch with the window shown in Figure 1, which allows the user to view, manipulate, or run the GCSolar.NET modeling simulation for photolysis of contaminants in water, as well as terminate the program. All user-modifiable variables are initialized with default values, provided in Appendix 1. Note to the user: this guide focuses on chemical contaminants, but the same steps can be used to compute values for biological contaminants. There are only two major differences. The first, and most important, is that no default values are provided for a biological contaminant. The user will need to input photolysis information either from experimental data or literature sources. This can be done in the same manner as inputting new photolysis data for a chemical contaminant, described below. The second difference is that instead of "Chemical Absorption Coefficient (L/(mole/cm))," biological contaminants use "Biological Weighting Function (hr^(-1) Watts^(-1) cm^2 nm)." If the user is reading this guide to use GCSolar.NET with a biological contaminant, simply keep these changes in mind. Simulations of inactivation of biological contaminants are described in more detail in a recent paper: "Biological weighting functions for evaluating the role of sunlight-induced inactivation of coliphages at selected beaches and nearby tributaries of the Great Lakes", R. G. Zepp, M. Molina, K. Wong, O. Georgacopoulos, B. Acrey, M. Cyterski, G. Whelan, R. Parmar". *The paper is Under internal review.*

There are three main windows in GCSolar.NET:

- View Current Values
- Modify Values
- Compute Photolysis

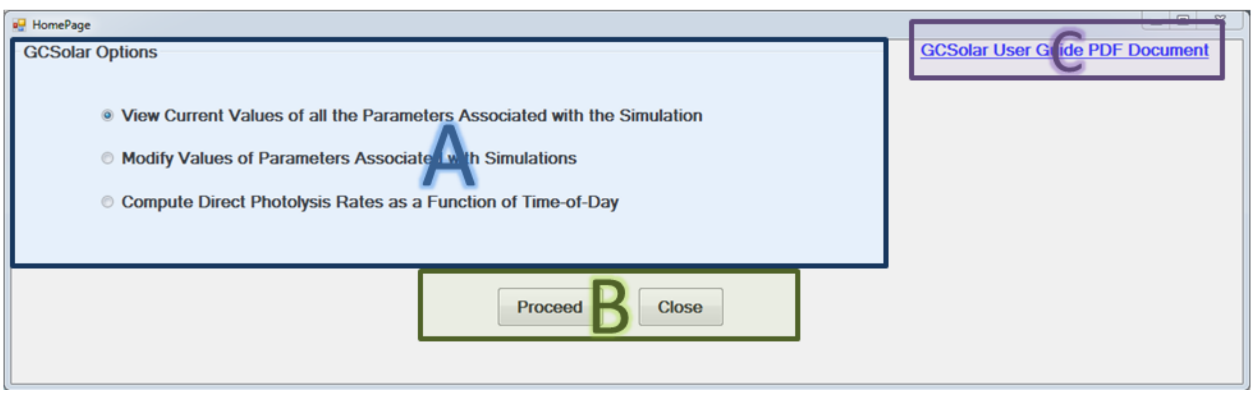

Figure 1. *The launch window has been divided into Section A, the radio buttons; Section B, the Proceed and Close buttons; and Section C, a link to this User Guide.*

Each of these windows can be selected via the radio buttons in Figure 1, **Section A**. Use of the radio buttons is discussed below, and each of these windows is discussed in detail in the following sections of this user guide.

Only one of the radio buttons can be selected at a given time. By default, the first option, View, is selected. To select a different option, click the corresponding radio button. Clicking a radio button will not advance the program to another window.

There are two buttons located at the bottom of this form in **Section B**, Proceed and Close.

- Proceed opens the next window.
- Close will exit the GCSolar.NET program.

Section C will open this User Guide.

Click Proceed to open the selected window.

2.1 View Current Values of all of the Parameters Associated with the Simulation

This window, shown in Figure 2, displays all user-editable values for the simulation.

> *Note: Values are not editable in this window. To edit, select the Close button and choose the "Modify" module instead, which is discussed in detail in 2.2, "Modify Values of Parameters Associated with Simulations."*

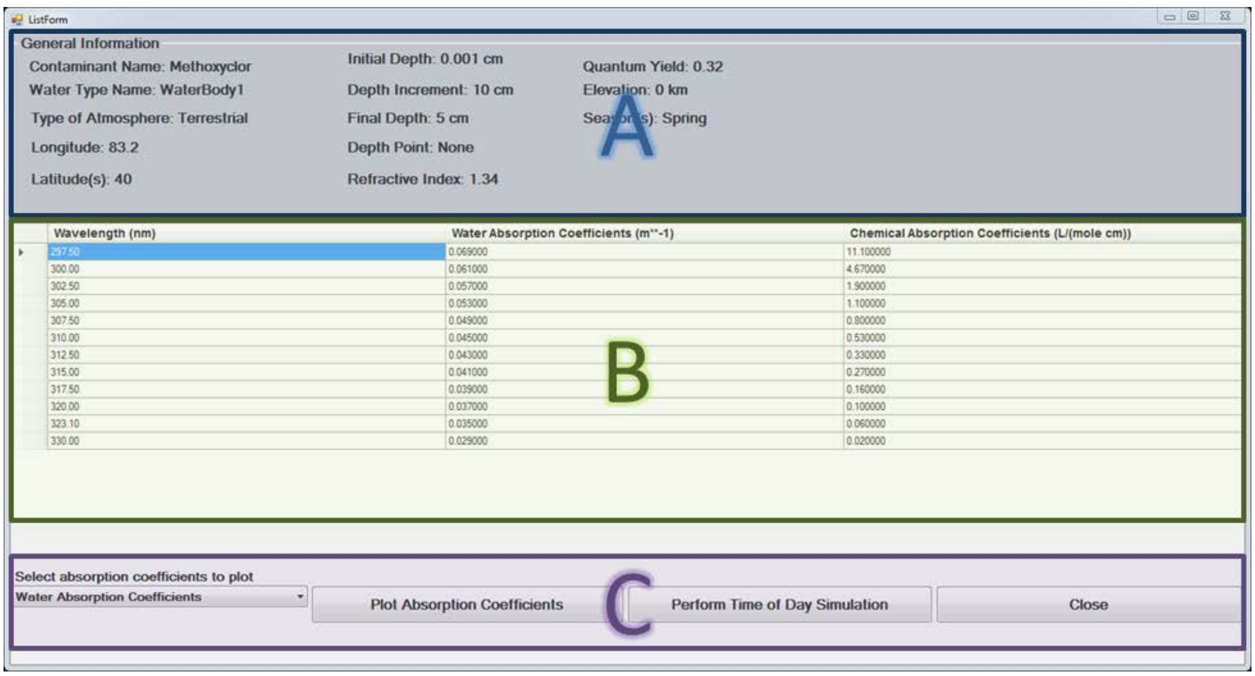

Figure 2. *The View Current Values window has been divided into Section A for parameters with a single value, such as water type; Section B for a table of wavelengths, water absorption coefficients, and contaminant absorption coefficients; and Section C for buttons to plot, run the simulation or close the current window and return to the launch window.*

Section A and **Section B** show the current values of parameters. **Section C** allows a choice via the drop-down menu at the far left to plot either of the following:

- Water Absorption Coefficients, shown in Figure 3
- Contaminant Absorption Coefficients, shown in Figure 4

To create an absorption plot, select the desired absorption coefficients to plot from the drop-down menu and click the Plot Absorption Coefficients button. As shown in Figures 3 and 4, this launches a new window with the absorption plot as well as buttons to Save Plot to File or

Close. Clicking Save Plot to File opens a standard Windows save dialogue by which the plot can be saved as a Portable Network Graphics (.PNG) file. As it does throughout this program, clicking Close closes the current window—in this case, the plot window—which leaves the parent window—in this case, the window for View Current Parameter Values—open.

Section C also has two other buttons, the Perform Time of Day Simulation button and the Close button.

- Click Perform Time of Day Simulation to run the model using current values of parameters, covered in more detail in 2.3, "Compute Direct Photolysis Rates as a Function of Time-of-Day."
- Click Close to close this window and return to the launch window. *Note: this does not exit the GCSolar.NET program.*

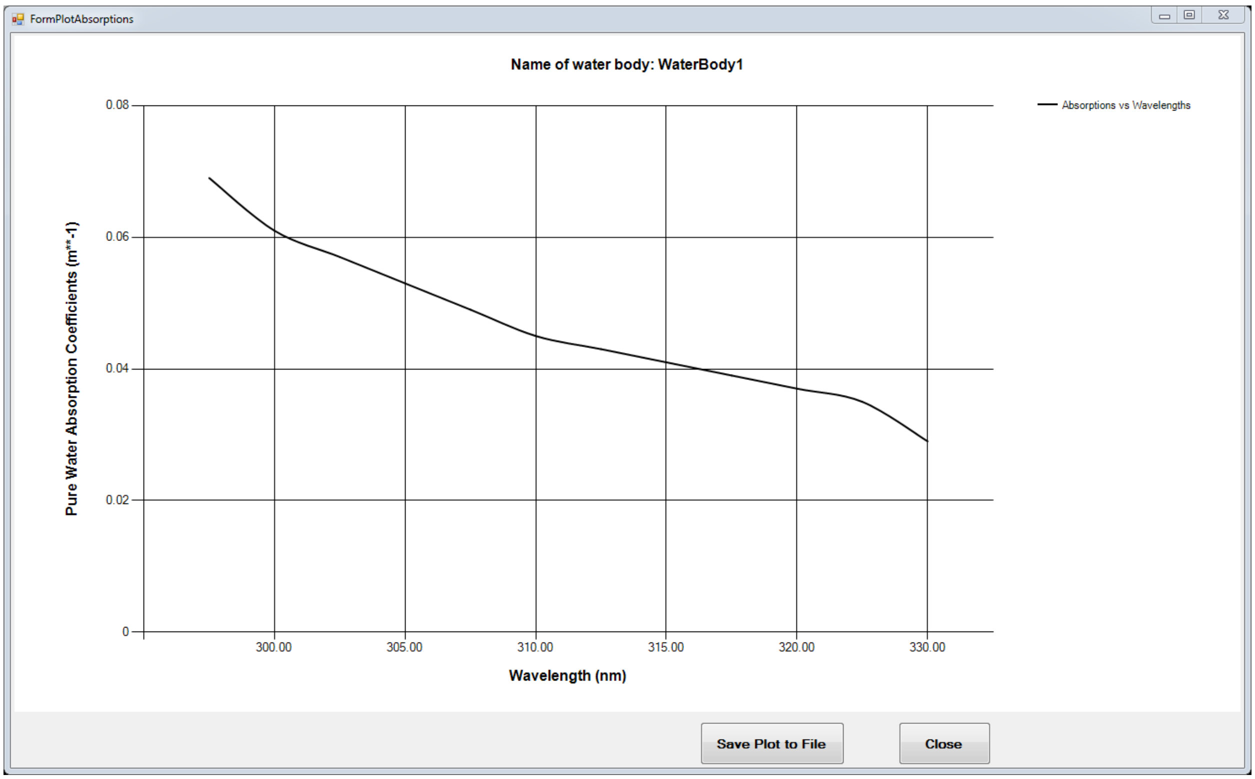

Figure 3. *This Water Absorption Coefficient plot is based on the default GCSolar.NET parameter values.*

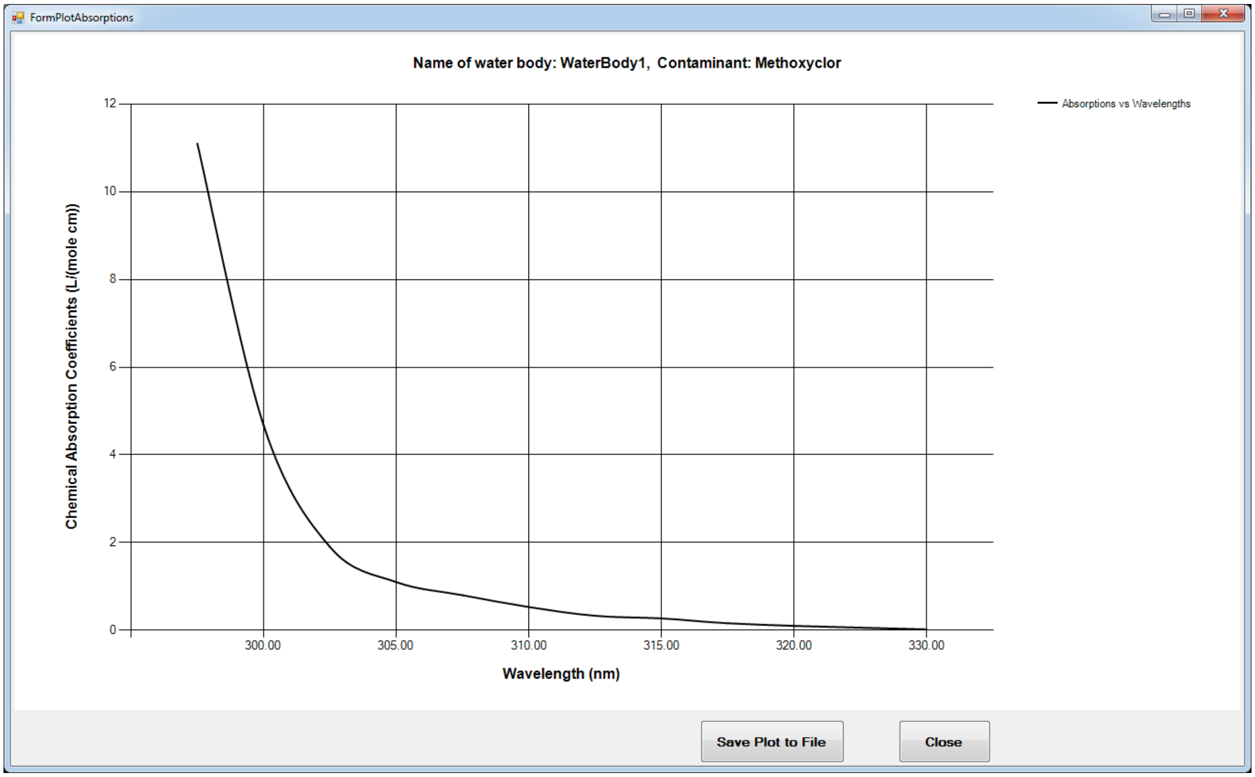

Figure 4. *This Contaminant Absorption Coefficient plot is based on the default GCSolar.NET parameter values.*

2.2 Modify Values of Parameters Associated with Simulations

This window, shown in Figure 5, can be used to edit parameter values of the simulation.

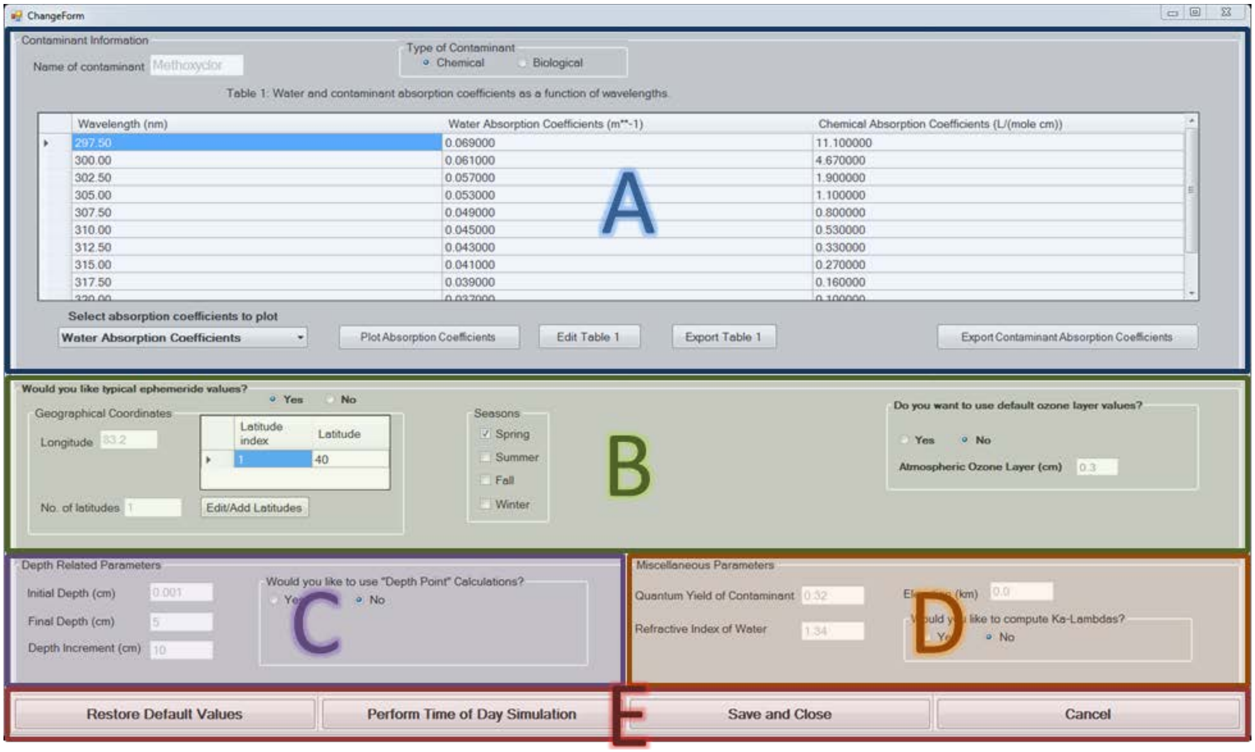

Figure 5. *The Modify Parameters window allows edits to contaminant-specific information (Section A), ephemeride values (Section B), depth-related parameters values (Section C), miscellaneous parameters values (Section D), and control buttons (Section E).*

Section A, Contaminant Information, includes the following:

- Name of Contaminant. *The contaminant name can be a string or one or more characters.*
- Type of Contaminant. *Choose chemical or biological using the radio buttons. A chemical contaminant can either be: a) a chemical that is toxic to plants and/or animal, and/or human beings, or b) a non-toxic chemical whose persistence is of interest in a body of water. A biological contaminant is a microorganism such as a bacterium or virus that is: a) pathogenic to plants and/or animals and/or human beings in a body of water, or b) a nonpathogenic proxy used as an indicator for a pathogen contaminant. Chemical is selected by default.* ***Note: Biological modeling results have not been verified yet.***
- Table: Wavelength, Water Absorption Coefficient, and Chemical Absorption Coefficient. To edit or export this table, use the four related buttons.
  - Click Edit Table 1 to launch a new window to edit the table. *See 2.2.1, "Edit Table 1 Form" for a full description of the edit table window.*
  - Click Export Table 1 to export the table to a comma-separated values (CSV) file. A standard Windows "Save As" dialogue box will appear allowing the user to choose a file name and location. Click the Save button to save the file, or the Cancel button to close the dialogue box without saving the file.
  - The Export Water Absorption Coefficients button functions similarly to

Export Table 1, except that it does not export the Chemical Absorption Coefficients column (only Wavelengths and Water Absorption Coefficients).

- The Export Contaminant Absorption Coefficients button functions similarly to Export Table 1, except that it does not export the Water Absorption Coefficients column (only Wavelengths and Chemical Absorption Coefficients).

Additionally, Contaminant Information contains a feature to plot the wavelength and coefficient data in the table. As with the plotting feature on the View window, discussed in 2.1, “View Current Values of all of the Parameters Associated with the Simulation,” either Water Absorption or Chemical Absorption can be plotted against wavelength; refer to 2.1 for a detailed description as well as plots of the default parameter values data set.

Click the Plot Absorption Coefficients button to generate a plot.

Section B contains entries and selections related to geographical and ephemeride coordinates, seasons, and ozone layer thickness. The first question in this section—“Would you like typical ephemeride values?”—controls the rest of the section. Selecting “No” sets this section to display different options than selecting “Yes,” as is shown in Figure 6.

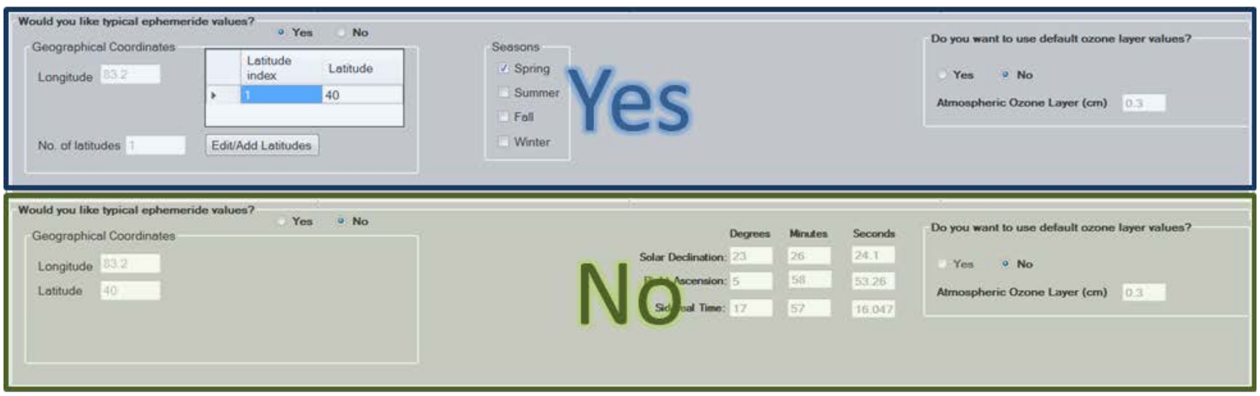

Figure 6. *The Modify Parameter values window, Section B, shown first in the “Yes” configuration (top), then the “No” configuration (bottom).*

- If the user selects “Yes,” the window is broken into “Geographical Coordinates,” “Seasons,” and “Do you want to use default ozone layer values?” data input areas.
  - Geographical Coordinates. *This contains the two editable areas, Longitude and Number of Latitudes, and one button,* Edit/Add Latitudes*. The table of latitude indices and latitudes is not directly editable; these values can be edited through the* Edit/Add Latitudes *button, discussed below.*
    - Longitude. *Enter a longitude in degrees. Values must be between -180 and 180.*
    - Number of latitudes. *Enter the number of latitudes to be used for the simulation. Values must be between 1 and 10; at least one latitude must be entered. Latitudes must be less than 70 when using typical ephemeride values. Once the number of latitudes has been entered, click the* Edit/Add Latitudes *button.*
    - The Edit/Add Latitudes button brings up a new window to edit the

table of latitude indices and latitudes. This table uses “Number of latitudes” to determine how many rows to create. Values for Latitude must be 0 or greater but less than 70 degrees. *For detailed instructions on editable tables in GCSolar.NET, see 2.2.2, “Enter Absorption Form.”*

  - Seasons. *Seasons contains four check boxes, one for each season. By default, “Spring” is checked. At least one season must be checked; up to four seasons may be checked.*
  - Do you want to use default ozone layer values? *If “Yes” is selected, no other choices are available. If “No” is selected, a text box will appear for the user to enter an atmospheric ozone layer thickness in centimeters (cm). Ozone thickness can be any non-negative numeric value.*
- If the user selects “No,” then Section B is broken into a different “Geographical Coordinates” subsection; a table for entering solar declination, right ascension, and sidereal time; and the same “Do you want to use default ozone layer values?” subsection.
  - Geographical Coordinates. *This contains two editable areas, longitude and latitude, both in degrees. Longitude must be between -180 and 180, and latitude must be between 0 and 70 (70 excluded).*
  - Solar Declination, Right Ascension, and Sidereal Time. *These parameters values are presented in tabular format, each having a row of three boxes for entering degrees, minutes, and seconds, respectively. Degrees must be between 0 and 90, and minutes and seconds must be between 0 and 60.*
  - Do you want to use default ozone layer values? *If “Yes” is selected, no other choices are available. If “No” is selected, a box will appear for the user to enter an atmospheric ozone layer thickness in cm. Ozone thickness can be any non-negative numeric value.*

Section C contains Depth Related Parameters. All four parameters can be directly edited in this window, have default values in gray text, and are in cm. Initial and final depth form the outer bounds of depth for the model, depth increment sets the interval, and depth point is an optional value which increases the layer thickness.

- Initial Depth. *Enter the shallowest depth in cm that will be used in calculation of photolysis rate constants. The default value is 0.001. This value must be greater than 0.*
- Final Depth. *Enter the deepest depth that will be used in the calculation of photolysis rate constants. The default value is 5 cm. This value must be greater than the initial depth.*
- Depth Increment. *This parameter defines how finely or coarsely the simulation calculates between the bounds of initial and final depth, i.e., for an increment of 1 and bounds of 1 and 3, the model will calculate depths of 1 cm, 2 cm, and 3 cm, whereas for a depth increment of 2, it would calculate only 1 cm and 3 cm.*
- Would you like to use “Depth Point” Calculations? *If “yes” is selected, this option computes the rate constant in a layer of thickness “delta depth” (cm) at a specified*

depth in a water body. Valid values are non-negative numbers. If "no" is selected, which is the default, the field for inputting depth point will disappear.

Section D is Miscellaneous Parameters. This section has three editable values and one yes/no radio button set. The editable values are Quantum Yield of Containment, Refractive Index of Water, and Elevation. "Would you like to compute Ka-Lambdas?" is a yes/no radio button.

- Quantum Yield of Containment. *This parameter has no units and is set to a default value of 0.32, which can be modified by the user. This value must be greater than zero and less than or equal to 1. This value represents the number of destroyed molecules divided by the number of photons absorbed by the system.*
- Refractive Index of Water. *This parameter has no units and is set to a default value of 1.34, which can be modified by the user. This value must be greater than one and less than four. This value represents the ratio of the speed of light in a vacuum to the speed of light in water.*
- Elevation. *Measured as kilometers (km) above sea level, this parameter has a default value of 0 km (sea level). This value can be modified by the user, and must be non-negative.*
- Would you like to compute Ka-Lambdas? *If the "yes" button is selected, then ka-lambdas will be calculated and included in GCSolar.NET's output. Ka-lambdas are sunlight absorption rate constants for the contaminant as a function of wavelength. "No" is the default.*

Section E has four buttons: Restore Default Values, Perform Time of Day Simulation, Save and Close, and Cancel.

- Clicking Restore Default Values resets all editable parameters to their default values. If no errors occur, a pop-up box will appear to say, "Input parameters were successfully set to their default values." ***Caution! This button will erase all changes.***
- Click Perform Time of Day Simulation to run the model. See 2.3, "Compute Direct Photolysis Rates as a Function of Time-of-Day" for more details. A pop-up will inform the user that "Parameters were successfully updated."
- Click Save and Close to save the currently entered parameter values and return to the Launch window. A pop-up will inform the user, "Parameters were successfully updated."
- Click Cancel button to close the Modify Values window without saving currently entered values and return to the Launch window. A pop-up will inform the user, "Exiting without saving any new changes." ***Note: The window will also close if the "X" button in the upper right of the form is clicked, as is standard for Windows. In this case, a pop-up will appear offering the user a chance to stay on the window and saying: Warning! No changes will be saved. Do you still want to close this window?***

2.2.1 Edit Table 1 Form

This section describes the pop-up window (Figure 7) that appears after clicking the

Edit Table 1 button seen in Section A of Figure 5.

Set the simulation's minimum and maximum wavelengths in **Section A** of this window. The default values are 297.5 and 330. Use only numerical characters (do not include the unit, which is nanometers) and follow the rules listed in **Section B**. Next, select the type of Water Body. By default, Natural Water is selected, and there is a space to enter the name of the water body. A name must be entered. If Pure Water is selected, the box for entering the name of the water body disappears. Click the Enter Absorption Data button after entering values for the minimum and maximum wavelengths and entering a name, if necessary, for the water body. This will launch a new pop-up to edit the wavelengths in the range between the selected minimum and maximum, covered in 2.2.2, "Enter Absorption Form."

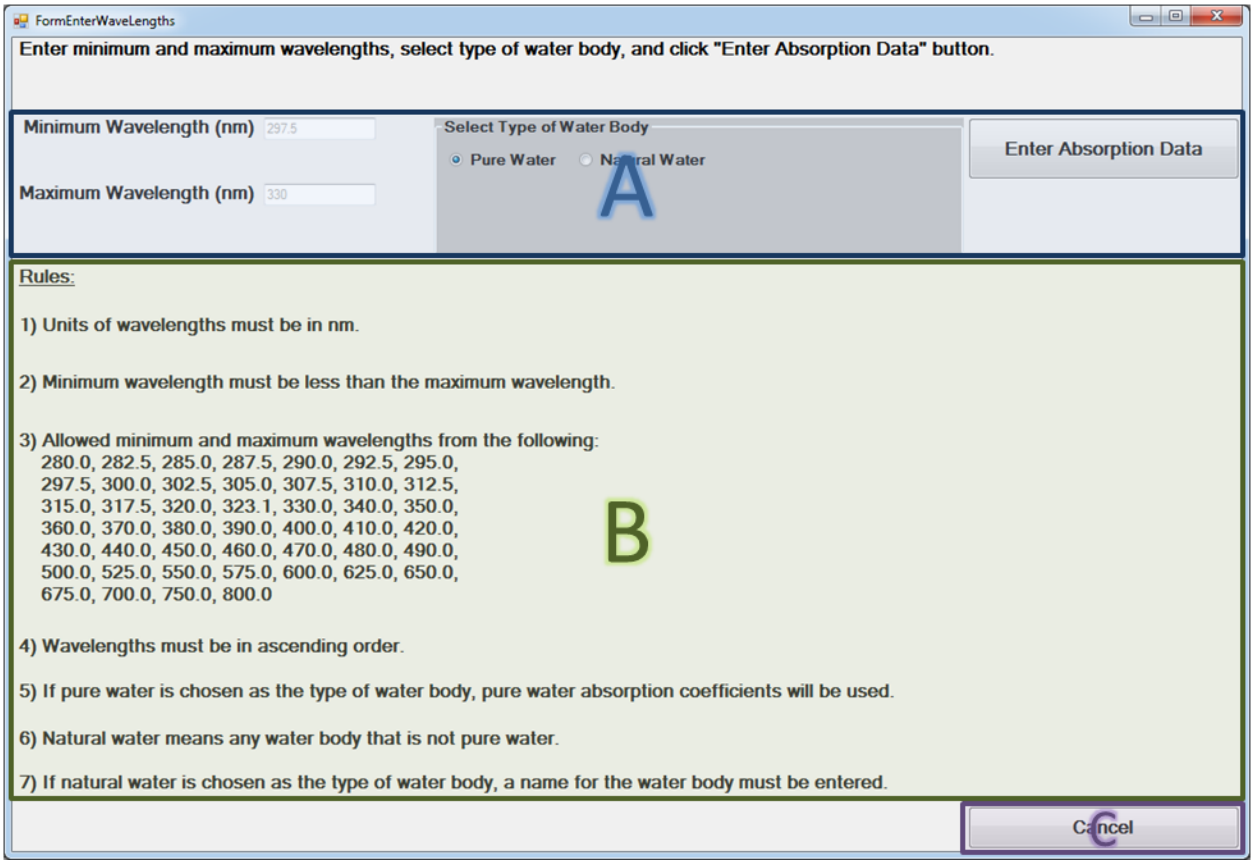

Figure 7. *This window allows the user to enter absorption coefficients for a range of wavelengths and choose the type of water body (Section A), provides instructions for how to enter valid data sets (Section B), and allows the user to close the Edit Table pop-up (Section C).*

Wavelengths less than 297.5 have little effect under usual environmental conditions. However, they are included in this modeling system because these wavelengths become very important determinants of photolysis for parts of the Earth where the ozone layer is strongly depleted.

The valid wavelengths are:

280	297.5	315	360	430	500	675
282.5	300	317.5	370	440	525	700
285	302.5	320	380	450	550	750
287.5	305	323.1	390	460	575	800
290	307.5	330	400	470	600	
292.5	310	340	410	480	625	
295	312.5	350	420	490	650	

Use the Cancel button in **Section C** to close this form and return to the Modify Values window.

2.2.2 Enter Absorption Form

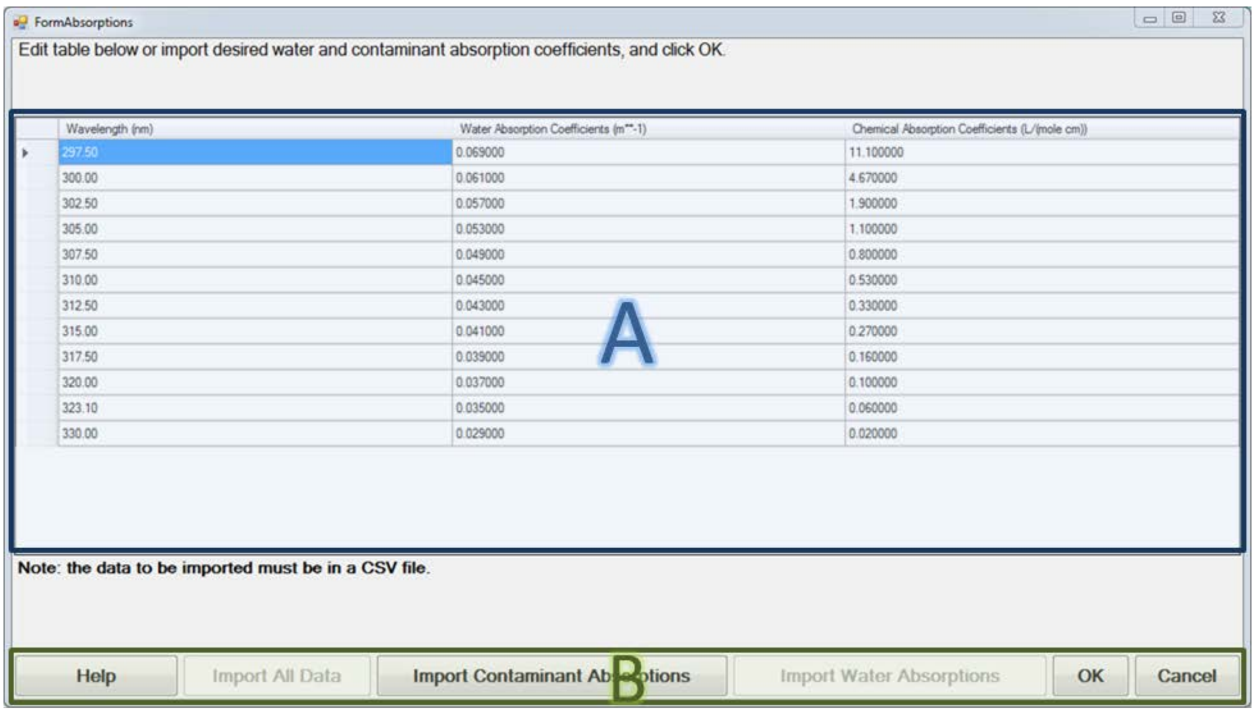

Figure 8. *This window allows the user to edit or import values for wavelengths, water absorption coefficients, and chemical absorption coefficients.*

Section A of Figure 8 is a table of wavelengths and their related water absorption coefficients and chemical absorption coefficients. The range of wavelengths listed in this table is determined by the previous window (Figure 7) and will be populated with default values for water absorption and chemical absorption. Any cell in water absorption or chemical absorption columns can be edited by clicking in the cell and entering a new value; wavelengths are not editable. Alternately, a set of new values can be imported, as is described below. If an invalid value is entered, a red error icon will appear to the left of the row being edited, as shown in Figure 9, and the user will be unable to select another cell until the error is corrected. Invalid values are: negative numbers, blanks, letters, or zeroes.

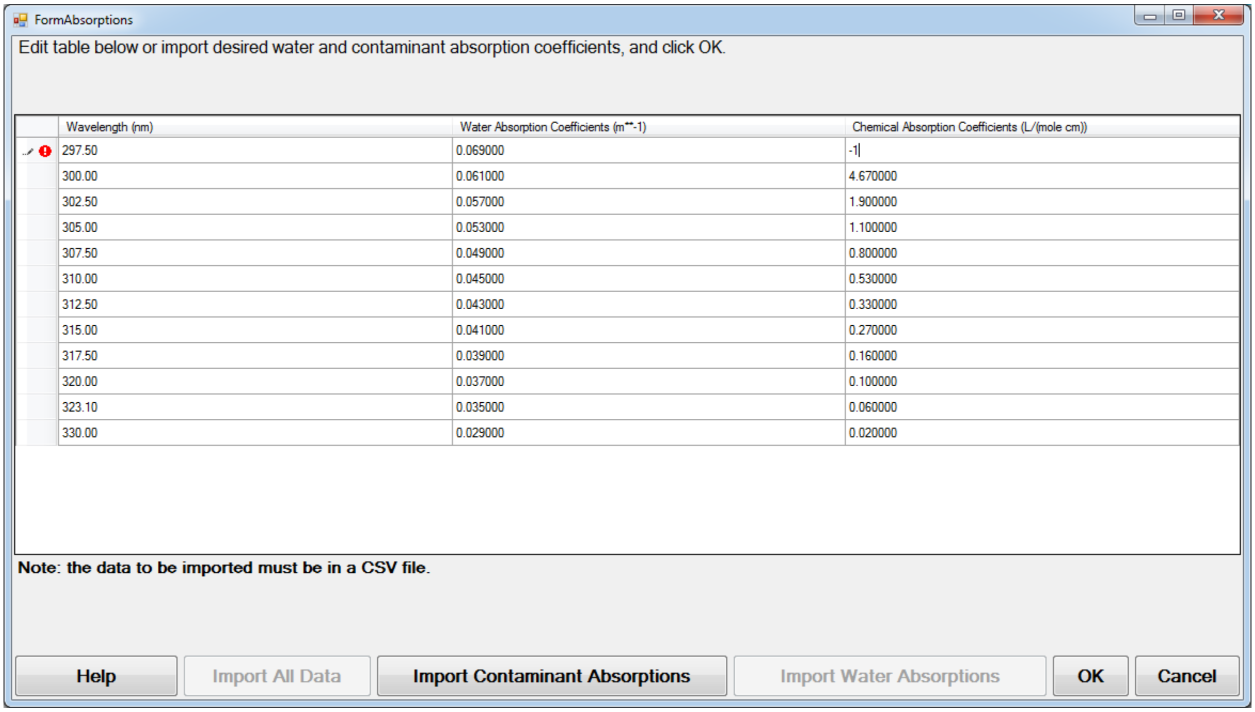

Figure 9. *If an invalid value such as a zero or negative number is entered, the form will display a red error icon to the left of the row being edited and no other cell can be selected until a valid value is entered. Water absorptions cannot be edited because pure water has been selected, so default values will be used.*

Section B of Figure 8 has six buttons.

- The Help button brings up a new window describing the data and assumptions. The Help window can be closed by scrolling to the bottom of the Help window and clicking the Close button.
- The Import All Data button imports a set of wavelengths, water absorption coefficients, and chemical absorption coefficients. The new data set must be in a .CSV file format and will completely replace the existing values. Clicking this button brings up a standard Windows dialogue box for opening a file. Navigate to and select the file, then click the Open button to import the file or the Cancel button to close the dialogue box.

  Note: To import values correctly, the CSV data must have column headers identical to those seen in GCSolar.NET, e.g., the wavelength column must have "Wavelength (nm)" in the first row.
- The Import Contaminant Absorptions button imports a list of chemical absorption coefficients. Like the Import All Data button, Import Contaminant Absorptions can accept a CSV file of values; the difference is that Import Contaminant Absorptions will import only wavelength and chemical absorption columns, and use existing water absorption coefficients. Like Import All Data, the CSV file must have headers identical to those in GCSolar.NET, and the chemical coefficients must be paired with wavelengths.
- The Import Water Absorptions button is the counterpart to the Import Contaminant

Absorptions button—it imports paired wavelengths and water absorption coefficients from a CSV file with headers identical to the GCSolar.NET Table 1 columns.

- The OK button saves the new values (a pop-up window will inform the user that "Data were successfully updated") and closes both the Enter Absorption and Edit Table 1 windows, returning the user to the Modify Parameters window shown in Figure 5 with updated parameters.
- The Cancel button also returns the user to the Modify Parameters window, but without having saved any edits.

2.3 Compute Direct Photolysis Rate Constants as a Function of Time-of-Day

This third and final module of GCSolar.NET runs the model. If no changes have been made through the "Modify Values of Parameters Associated with Simulations" (Figure 5), this will be run with default values of parameters. The model can be run via this command from the launch window (Figure 1), or using the Perform Time of Day Simulation button available in either of the previous two modules. The model will function the same way regardless of how it is reached, excepting the ka-lamda table, which will not appear unless ka-lambdas were enabled in the Modify Values window (the "Would you like to compute Ka-Lambdas?" control; see Section 2.2, Modify Values of Parameters Associated with Simulations).

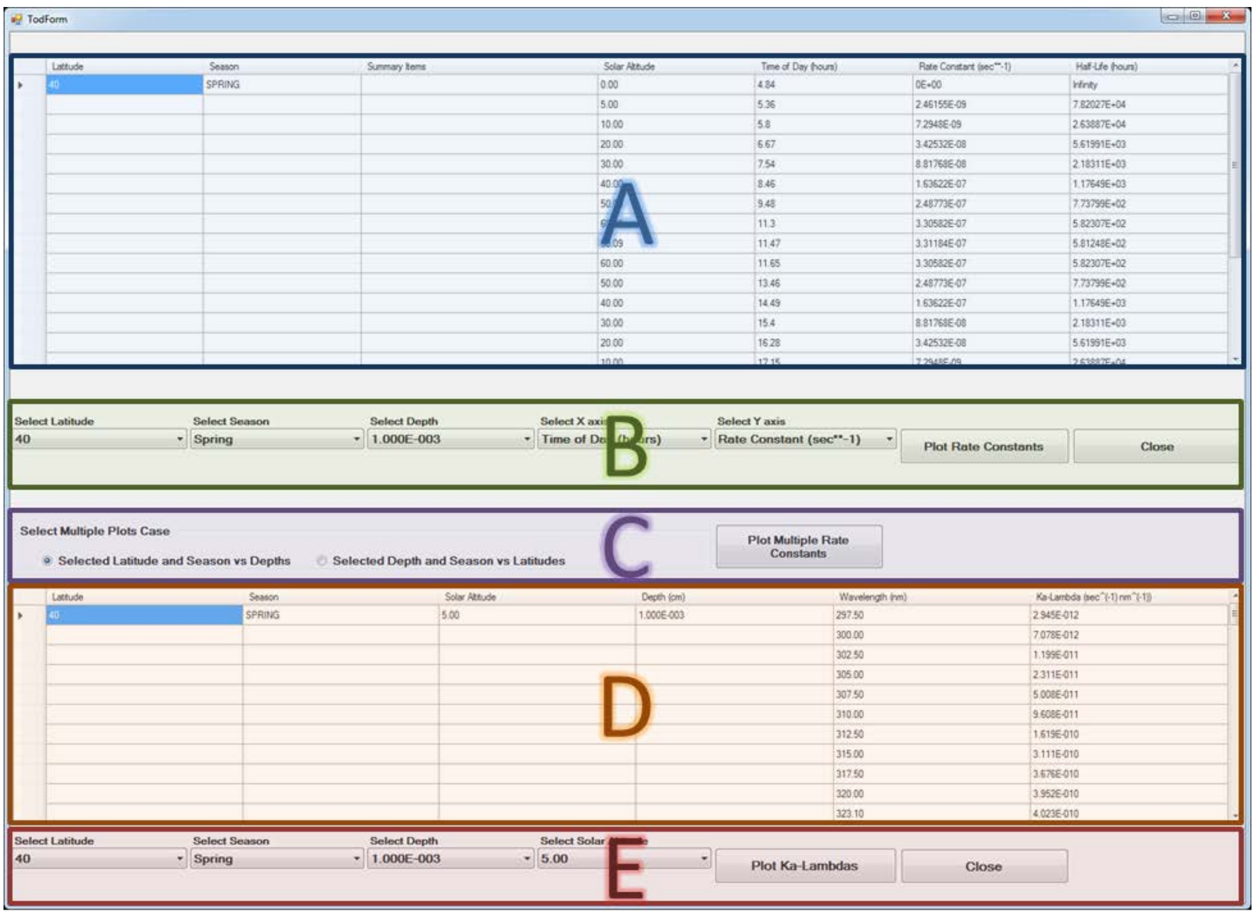

Figure 10. *This window allows the user to view (Section A) and plot (Section B) the outputs of the*

GCSolar.NET photolysis model, or close this pop-up window. The user can view (Section D) and plot (Section E) the ka-lamda values. Section C allows the user to plot multiple rate constants on the same graph.

Section A of Figure 10 is a table of values generated by the model based on the parameters (either default or user-input). This table cannot be edited by the user. The columns are:

- Latitude. *The latitudes are set in "Geographical Coordinates" on the Modify Values window.*
- Season. *The seasons are selected under "Would you like typical ephemeride values? (Yes)" on the Modify Values window.*
- Summary Items. *Includes Depth (cm), Depth Point (cm), Average Rate Constant(sec**-1), Integrated Rate Constant(day**-1), and Integrated Half-Life (days). Displayed in the rows (i.e., one item per row) below the last row of data. Depth and Depth Point are set by the user in previous windows or left at default; Average Rate Constant, Integrated Rate Constant and Integrated Half-Life are produced by the GCSolar.NET model.*
- Solar Altitude, Time of Day (hours), Rate Constant (sec**-1), Half Life (hours). *These values are produced by the GCSolar.NET model based on the parameters entered or default values.*

Section B of Figure 10 provides a variety of options for plotting the model output data shown in Section A. There are five drop-down menus controlling what data is plotted, or four if non-default ephemeride values were selected, and a button for generating the plot.

- Select Latitude. *This drop-down menu will present all latitudes input under "Geographical Coordinates" on the Modify Values window.*
- Select Season. *This drop-down menu will appear only if typical ephemeride values were used. (Non-default ephemeride values do not present an option to select a season.) If it is present, it will present all seasons selected on the Modify Values window.*
- Select Depth. *This drop-down menu will present all depths analyzed in this model run. This is determined by "Depth Related Parameters" on the Modify Values window.*
- Select X axis. *This can be **Time of Day (hours)** or **Solar Altitude**.*
- Select Y axis. *This can be only **Rate Constant (sec**-1)**.*
- Click the [Plot Rate Constants] button to generate a plot with the selected attributes.
- Click [Close] to close this window.

Section C is the "Select Multiple Plots Case" window, and allows multiple datasets to be visualized together. Select one of the radio button options and click the Plot Multiple Rate Constants button to launch a plot window, much like the Plot Rate Constants button in Section B. Like with previously described plots, the plot window will have buttons to export the plot or close the window. The two plotting options are:

- Selected Latitude and Season vs Depths. *This will plot multiple depths for the selected latitude and season, as shown in Figure 11.*

- Select Depth and Season vs Latitudes. *This will plot multiple latitudes for the selected depth and season, as shown in Figure 11.*

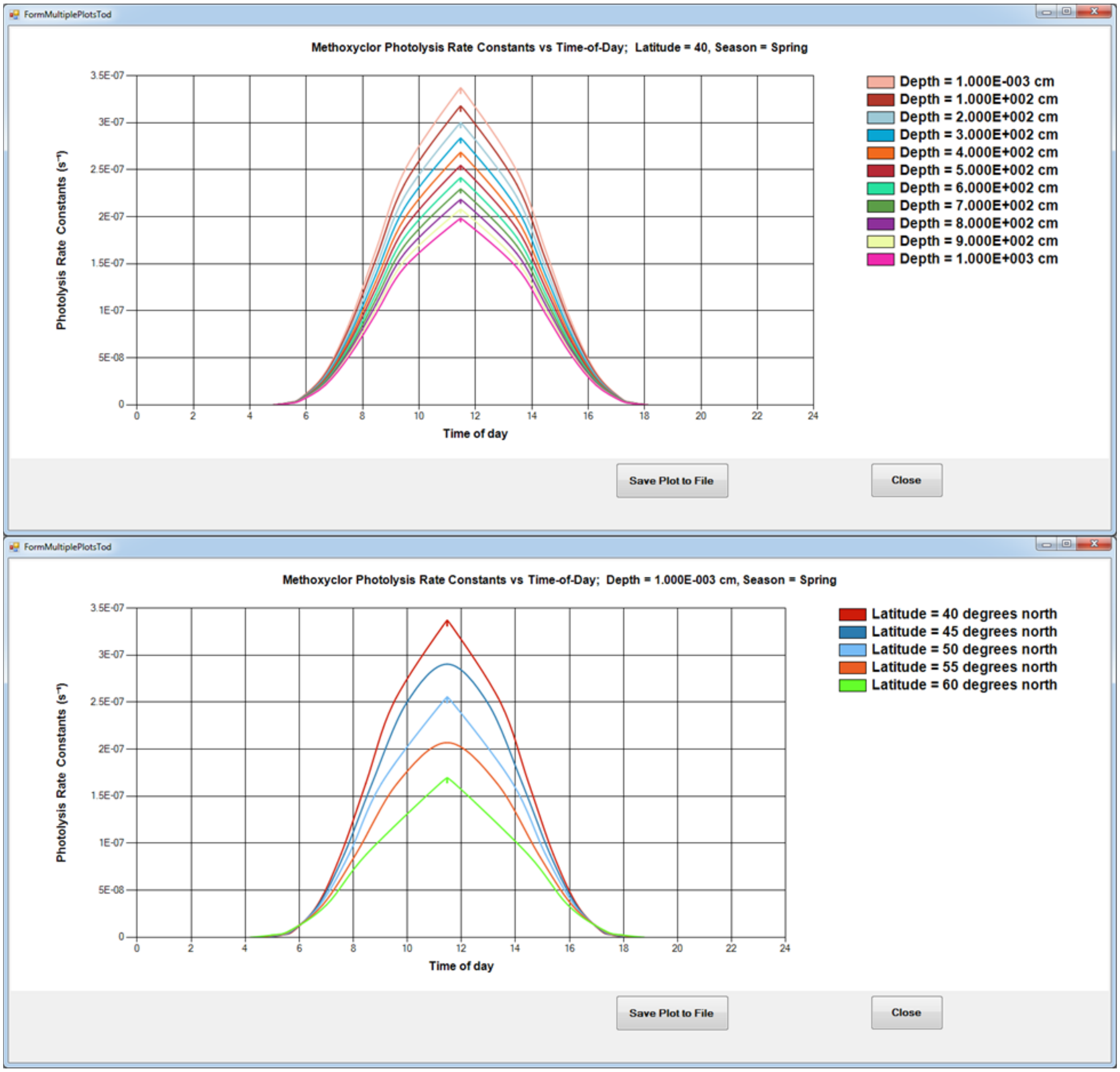

Figure 11. *Multiple Rate Constant plots for multiple depths (top) and multiple latitudes (bottom).*

Section D and **Section E** of Figure 10 are related to the ka-lambda values and as such will appear on this window only if "**Would you like to compute Ka-Lambdas?**" is set to "Yes" on the Modify Values window. If they are present, then Section C will present the ka-lambda values and Section D will provide plotting controls similar to Sections A and B above.

Section C is a table of ka-lambda and associated values that cannot be edited by the user with the following columns:

- Latitude. *The latitudes are set in "Geographical Coordinates" on the Modify Values window.*
- Season. *The seasons are selected under "Would you like typical ephemeride*

values? (Yes)" on the Modify Values window.

- Solar Altitude. *This value is produced by the GCSolar.NET model based on the parameters entered.*
- Depth (cm). *The depths calculated are determined by "Depth Related Parameters" on the Modify Values window.*
- Wavelength (nm). *The wavelengths are entered in the table under "Contaminant Information" on the Modify Values window.*
- Ka-Lambda (sec^(-1)nm^(-1)). *This value is produced by the GCSolar.NET model based on the parameters entered.*

Section D provides a variety of options for plotting ka-lambda values. There are four drop-down menus, or three if non-default ephemeride values were selected, and a button for generating the plot.

- Select Latitude. *This drop-down menu will present all latitudes input under "Geographical Coordinates" on the Modify Values window.*
- Select Season. *This drop-down menu will appear only if typical ephemeride values were used (non-default ephemeride values do not present an option to select a season). If it is present, it will present all seasons selected on the Modify Values window.*
- Select Depth. *This drop-down menu will present all depths analyzed in this model run. This is determined by "Depth Related Parameters" on the Modify Values window.*
- Select Solar Altitude. *This drop-down menu will present all solar altitudes calculated for this set of parameters.*
- Click the Plot Ka-Lambdas button to generate a plot with the selected attributes.
- Click Close to close this window.

3.0 Sample Session

Chapter 3 presents a walkthrough for using the GCSolar.NET program to analyze the potential chemical contaminants Methoxyclor and Carbazole. This walkthrough assumes that the user has read through Chapter 2 and can therefore navigate the various modules of the GCSolar.NET program. This walkthrough is presented in six parts below, each of which builds on the edits of the previous part and focuses on editing a different aspect of the data set. Throughout the walkthrough, example outputs are shown to check progress and compare how changing parameters affects the output. *Note: tables and plots can be exported, but other input data (such as ozone layer thickness) cannot be saved between sessions.*

3.1 PART I: Basic Modifications

1. Open GCSolar.NET
2. From the launch window, open the View module to see what default values are in use
3. Close the View module
4. From the launch window, select and open the Modify Values module to begin setting up the scenario. See Figure 12 for reference.

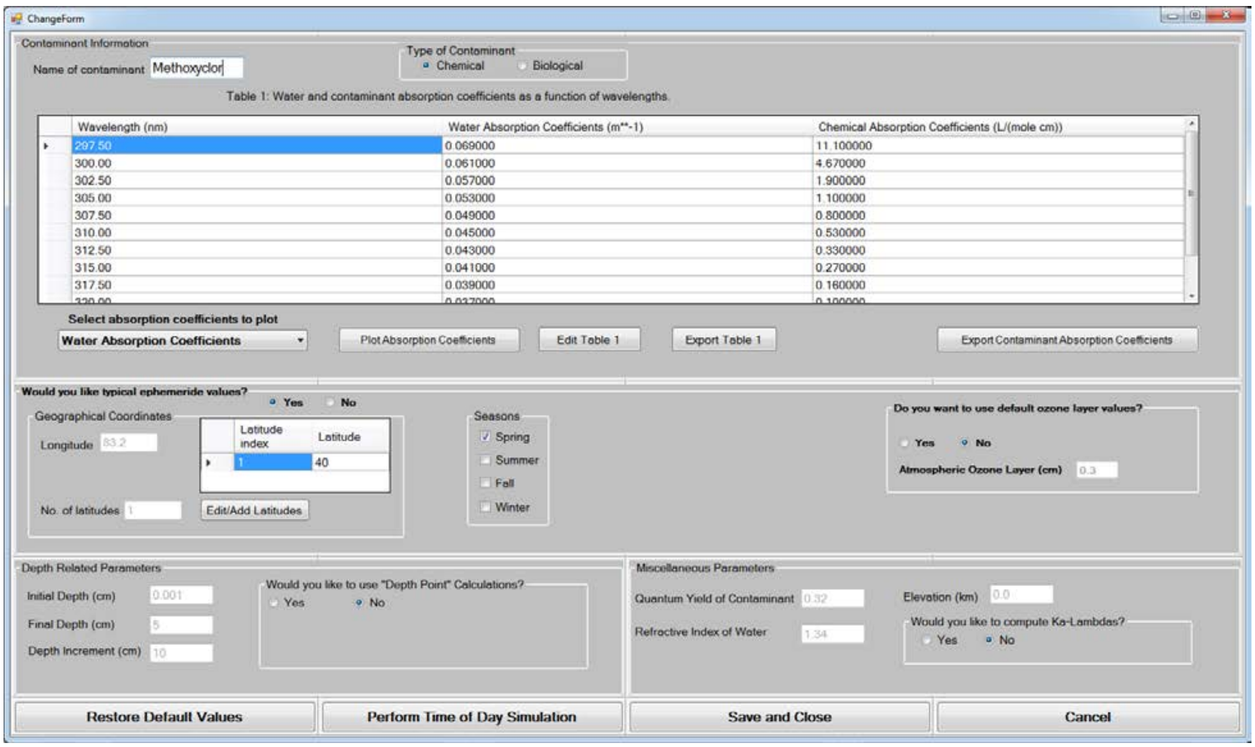

Figure 12. *The Modify Values module shown with the changes made in Part I of this walkthrough.*

a. Under "Contaminant Information"
   i. Enter the **Name of contaminant**: Methoxyclor
   ii. Select the **Type of Contaminant**: Chemical *(default)*
   iii. Click the Edit Table 1 button to select wavelength range and set coefficients.
      1. Set the **Minimum Wavelength (nm)**: 280.0

2. Set the **Maximum Wavelength (nm)**: 330.0
3. Select **Type of Water Body**: Pure Water
4. Click the Enter Absorption Data button
5. Click the OK button, accepting the default values.
   a. *A pop-up should inform the user, "Data were successfully updated." Click OK to continue.*

b. Under "Would you like typical ephemeride values?"

i. Set **Would you like typical ephemeride values?** to: Yes *(default)*

ii. Under "Geographical Coordinates"

1. Set **Longitude**: 90.0
2. Set **No. of latitudes**: 1
3. Click the Edit/Add button, and set **Latitude**: 40
   a. *A pop-up should inform the user, "Latitudes were successfully entered." Click OK to continue.*

iii. Under "Seasons"

1. Select **Spring** *(default)*

iv. Under "Do you want to use default ozone layer values?"

1. Set **Do you want to use default ozone layer values?** to: Yes

c. Under "Depth Related Parameters"

1. Leave default values

d. Under "Miscellaneous Parameters"

1. Leave default values

5. Click the Perform Time of Day Simulation button to run the model. *A pop-up should inform the user, "Parameters were successfully updated."* Figure 13 shows the model output for this scenario, also provided in tabular format below.

Latitude	Season	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
40	SPRING		0.00	5.29	0E+00	Infinity
			5.00	5.81	2.17687E-09	8.84296E+04
			10.00	6.25	6.35273E-09	3.03019E+04
			20.00	7.12	2.93284E-08	6.5636E+03
			30.00	7.99	7.49012E-08	2.57005E+03
			40.00	8.91	1.38053E-07	1.3944E+03
			50.00	9.93	2.08949E-07	9.21278E+02
			60.00	11.75	2.77389E-07	6.9397E+02
			60.09	11.92	2.779E-07	6.92696E+02
			60.00	12.1	2.77389E-07	6.9397E+02
			50.00	13.92	2.08949E-07	9.21278E+02
			40.00	14.94	1.38053E-07	1.3944E+03

Latitude	Season	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
			30.00	15.85	7.49012E-08	2.57005E+03
			20.00	16.73	2.93284E-08	6.5636E+03
			10.00	17.6	6.35273E-09	3.03019E+04
			5.00	18.04	2.17687E-09	8.84296E+04
			0.00	18.55	0E+00	Infinity
		Depth (cm) = 1.000E-003				
		Depth Point (cm) = None				
		Average Rate Constant (sec**-1) = 1.27E-07				
		Integrated Rate Constant (day**-1) = 6.06E-03				
		Integrated Half-Life (days) = 1.14E+02				

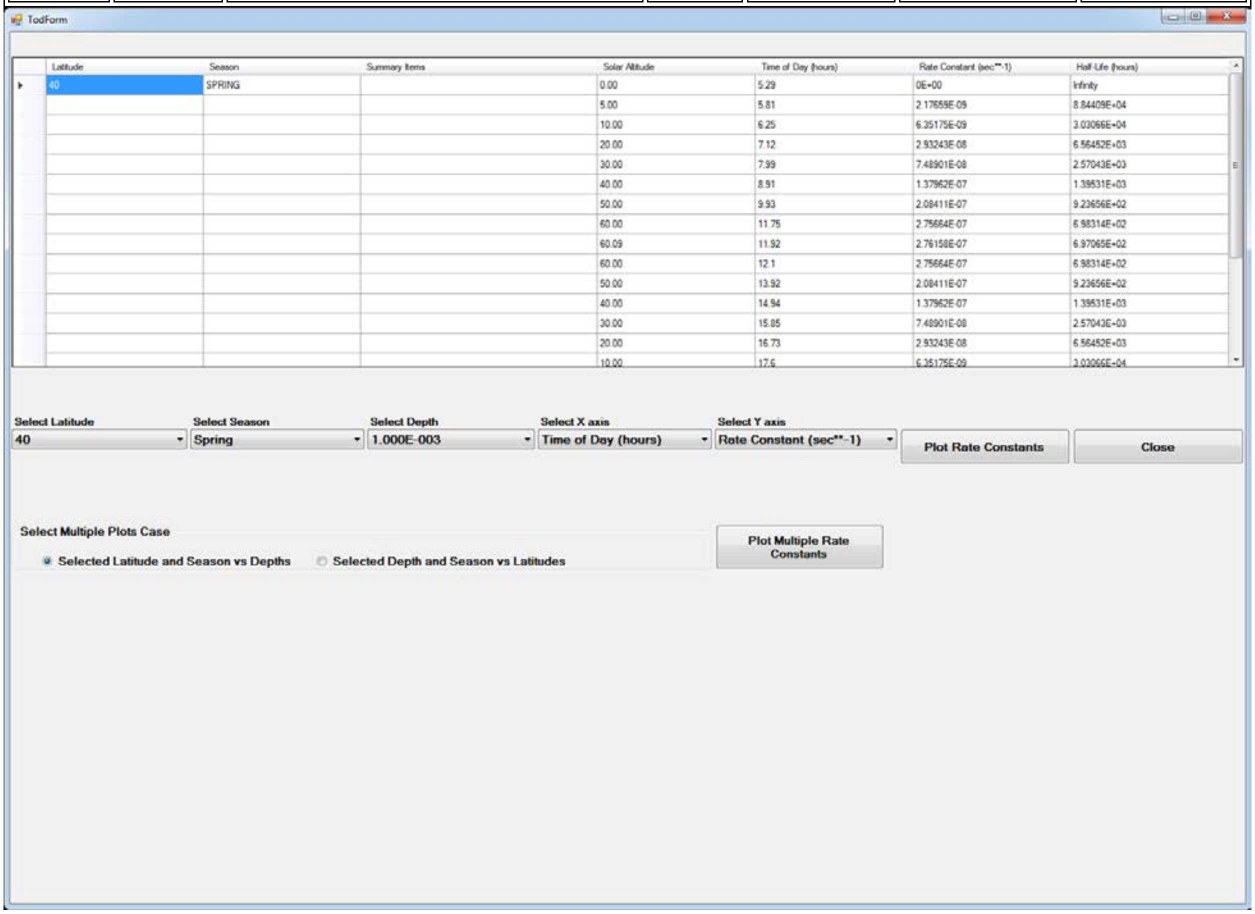

Figure 13. *The model output shown with the changes made in Part I of this walkthrough.*

6. Set the plotting parameters below the output table as follows:
   a. **Select Latitude**: 40 *(default)*
   b. **Select Season**: Spring *(default)*

c. **Select Depth**: 1.000E-003 *(default)*

d. **Select X axis**: Time of Day (hours) *(default)*

e. **Select Y axis**: RATE CONSTANT (sec**-1) *(default)*

7. Click the Plot Rate Constants button to generate a plot of the output, shown in Figure 14

8. Click the Save Plot to button on the plot output window to save the plot as a .PNG file using a standard Windows form

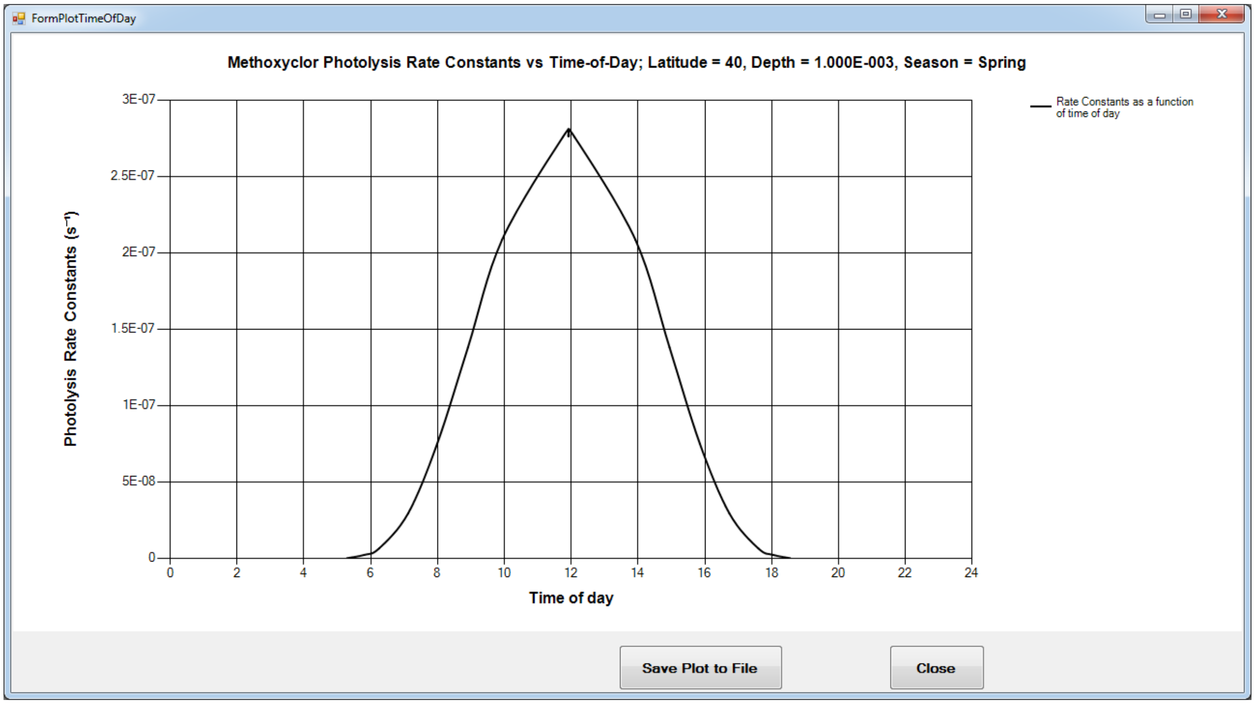

Figure 14. *The Time of day vs. Photolysis Rate Constant plot as generated in Part I.*

9. Click the Close button to close the plot window

10. Click the Close button to close the output window

3.2 PART II: Changing Elevation and Ozone

11. From the Modify Values module, under "Do you want to use default ozone layer values?"

a. Set **Do you want to use default ozone layer values?** to: No

i. Set **Atmospheric Ozone Layer (cm)**: 0.200

b. Click the Perform Time of Day Simulation button. The results are shown below, and plotted in Figure 15. Compare these values to those generated under Part I to see the difference caused by the change to ozone layer thickness. This distinction is demonstrated in Figure 16.

Latitude	Season	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
40	SPRING		0.00	5.29	0E+00	Infinity
			5.00	5.81	3.3547E-09	5.73821E+04
			10.00	6.25	1.0316E-08	1.86604E+04
			20.00	7.12	5.07091E-08	3.79616E+03
			30.00	7.99	1.35676E-07	1.41882E+03
			40.00	8.91	2.64659E-07	7.27351E+02
			50.00	9.93	4.26772E-07	4.5106E+02
			60.00	11.75	6.01517E-07	3.20024E+02
			60.09	11.92	6.02942E-07	3.19268E+02
			60.00	12.1	6.01517E-07	3.20024E+02
			50.00	13.92	4.26772E-07	4.5106E+02
			40.00	14.94	2.64659E-07	7.27351E+02
			30.00	15.85	1.35676E-07	1.41882E+03
			20.00	16.73	5.07091E-08	3.79616E+03
			10.00	17.6	1.0316E-08	1.86604E+04
			5.00	18.04	3.3547E-09	5.73821E+04
			0.00	18.55	0E+00	Infinity
		Depth (cm) = 1E-03				
		Depth Point (cm) = None				
		Average Rate Constant (sec**-1) = 2.59E-07				
		Integrated Rate Constant (day**-1) = 1.24E-02				
		Integrated Half-Life (days) = 5.6E+01				

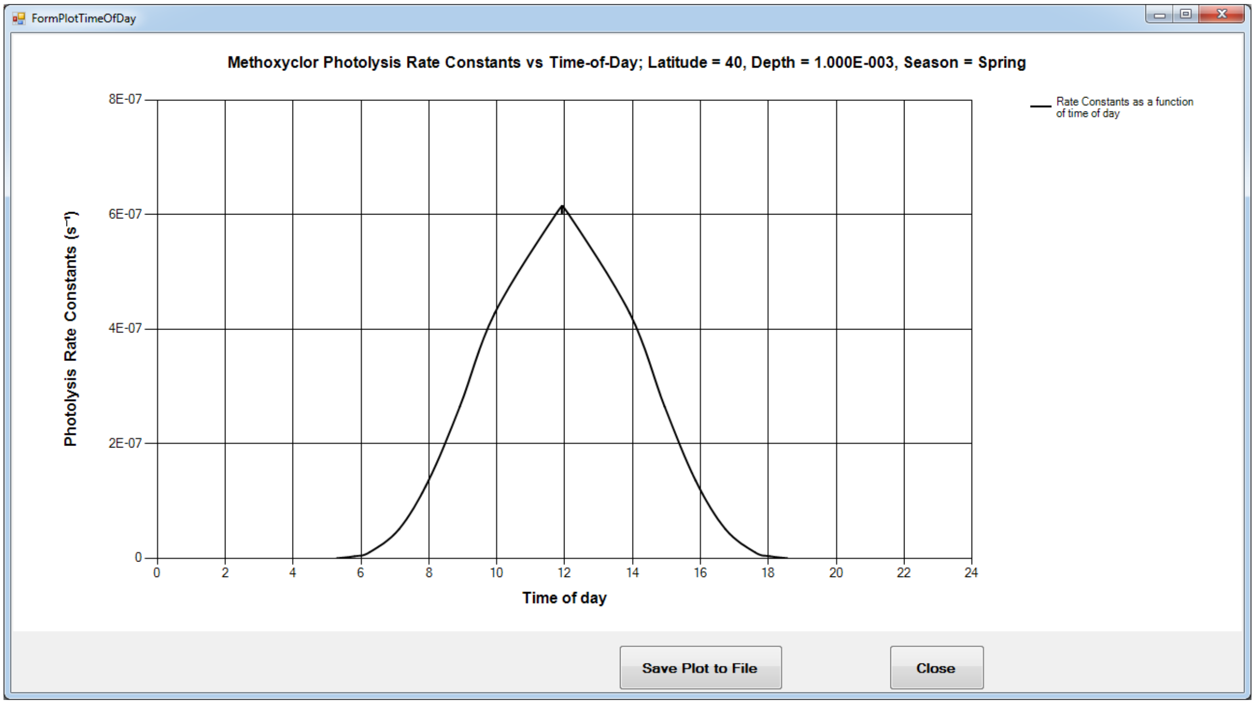

Figure 15. *The Time of day vs. Photolysis Rate Constant plot as generated by changing Ozone Layer Thickness to 0.200.*

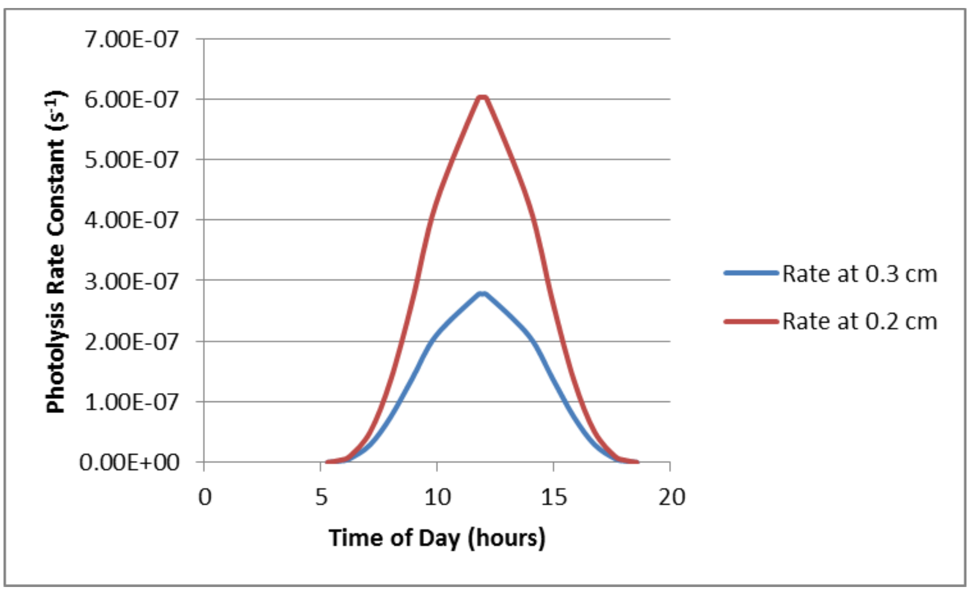

Figure 16. *Comparison of Photolysis Rate Constants for Ozone Thicknesses of 0.3 cm and 0.2 cm (graph generated in Microsoft Excel using GCSolar output data).*

12. Close the plotting and output windows
13. Under "Do you want to use default ozone layer values?"
    a. Set **Do you want to use default ozone layer values?** to: Yes
14. Under "Miscellaneous Parameters"
    a. Set **Elevation (km)**: 4.0

15. Click Perform Time of Day Simulation. Model output for this elevation is shown below.

Latitude	Season	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
40	SPRING		0.00	5.29	0E+00	Infinity
			5.00	5.81	1.846E-09	1.04279E+05
			10.00	6.25	6.11377E-09	3.14863E+04
			20.00	7.12	3.7138E-08	5.18337E+03
			30.00	7.99	1.02368E-07	1.88048E+03
			40.00	8.91	1.89893E-07	1.01373E+03
			50.00	9.93	2.84953E-07	6.75549E+02
			60.00	11.75	3.74798E-07	5.1361E+02
			60.09	11.92	3.7546E-07	5.12705E+02
			60.00	12.1	3.74798E-07	5.1361E+02
			50.00	13.92	2.84953E-07	6.75549E+02
			40.00	14.94	1.89893E-07	1.01373E+03
			30.00	15.85	1.02368E-07	1.88048E+03
			20.00	16.73	3.7138E-08	5.18337E+03
			10.00	17.6	6.11377E-09	3.14863E+04
			5.00	18.04	1.846E-09	1.04279E+05
			0.00	18.55	0E+00	Infinity
		Depth (cm) = 1E-03				
		Depth Point (cm) = None				
		Average Rate Constant (sec**-1) = 1.72E-07				
		Integrated Rate Constant (day**-1) = 8.21E-03				
		Integrated Half-Life (days) = 8.45E+01				

16. Close the plotting and output windows
17. Reset the altitude to 0.0

3.3 PART III: Changing Latitude, and Season, and Contaminant Absorption

18. From the Modify Values module, under "Contaminant Information"
    a. Set **Name of contaminant**: Carbazole
    b. Click Edit Table 1
        i. Set **Minimum Wavelength**: 297.5
        ii. Set **Maximum Wavelength**: 390.0
        iii. Set **Select Type of Water Body**: Pure Water
        iv. Click Enter Absorption Data

1. Set the **Chemical Absorption Coefficients (L/(mole cm))** to the following values:

   Wavelength (nm)--------- Chemical Absorption Coefficients (L/(mole cm))

   297.50 --------------------- 5540

   300.00 --------------------- 3100

   302.50 --------------------- 2440

   305.00 --------------------- 2270

   307.50 --------------------- 2390

   310.00 --------------------- 2530

   312.50 --------------------- 2600

   315.00 --------------------- 2700

   317.50 --------------------- 2920

   320.00 --------------------- 3190

   323.10 --------------------- 3170

   330.00 --------------------- 2900

   340.00 --------------------- 1520

   350.00 --------------------- 166

   360.00 --------------------- 23

   Wavelength (nm)--------- Chemical Absorption Coefficients (L/(mole cm))

   370.00 --------------------- 13

   380.00 --------------------- 12

   390.00 --------------------- 2

2. Click OK

   a. *A pop-up should inform the user, "Data were successfully updated." Click OK to continue.*

19. Under "Would you like typical ephemeride values?"

    a. Under "Geographical Coordinates"

       i. Set **No. of latitudes**: 2

       ii. Click Edit/Add

          1. Set the following values:

             Latitude index ------------ Latitude

             1 ---------------------------- 30

             2 ---------------------------- 50

             a. *A pop-up should inform the user, "Latitudes were successfully entered." Click OK to continue.*

    b. Under "Seasons"

       i. Check **Summer** and **Winter** only

20. Under "Miscellaneous Parameters"

    a. Set **Quantum Yield of Contaminant**: 0.0033

21. Click Perform Time of Day Simulation. Model output at this point is below.

Latitude	Season	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
30	SUMMER		0.00	5.13	0E+00	Infinity
			5.00	5.61	3.0716E-06	6.2671E+01
			10.00	6.01	7.08071E-06	2.71865E+01
			20.00	6.81	2.24044E-05	8.59206E+00
			30.00	7.59	4.34114E-05	4.43432E+00
			40.00	8.36	6.48118E-05	2.97014E+00
			50.00	9.13	8.34518E-05	2.30672E+00
			60.00	9.9	9.81039E-05	1.96221E+00
			70.00	10.71	1.08485E-04	1.77444E+00
			80.00	11.89	1.14644E-04	1.6791E+00
			80.09	11.99	1.14664E-04	1.67882E+00
			80.00	12.09	1.14644E-04	1.6791E+00
			70.00	13.27	1.08485E-04	1.77444E+00
			60.00	14.08	9.81039E-05	1.96221E+00
			50.00	14.85	8.34518E-05	2.30672E+00
			40.00	15.62	6.48118E-05	2.97014E+00
			30.00	16.39	4.34114E-05	4.43432E+00
			20.00	17.17	2.24044E-05	8.59206E+00
			10.00	17.96	7.08071E-06	2.71865E+01
			5.00	18.37	3.0716E-06	6.2671E+01
			0.00	18.85	0E+00	Infinity
		Depth (cm) = 1.000E-003				
		Depth Point (cm) = None				
		Average Rate Constant (sec**-1) = 6.36E-05				
		Integrated Rate Constant (day**-1) = 3.14E+00				
		Integrated Half-Life (days) = 2.2E-01				
30	WINTER		0.00	6.84	0E+00	Infinity
			5.00	7.33	3.08775E-06	6.23431E+01
			10.00	7.77	7.12037E-06	2.70351E+01
			20.00	8.7	2.25318E-05	8.54348E+00
			30.00	9.8	4.36479E-05	4.4103E+00
			39.86	12.08	6.48538E-05	2.96821E+00
			30.00	14.36	4.36479E-05	4.4103E+00
			20.00	15.46	2.25318E-05	8.54348E+00
			10.00	16.39	7.12037E-06	2.70351E+01
			5.00	16.83	3.08775E-06	6.23431E+01
			0.00	17.32	0E+00	Infinity

Latitude	Season	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
		Depth (cm) = 1.000E-003				
		Depth Point (cm) = None				
		Average Rate Constant (sec**-1) = 3.5E-05				
		Integrated Rate Constant (day**-1) = 1.32E+00				
		Integrated Half-Life (days) = 5.24E-01				
50	SUMMER		0.00	4.18	0E+00	Infinity
			5.00	4.88	2.99376E-06	6.43003E+01
			10.00	5.44	6.88953E-06	2.79409E+01
			20.00	6.5	2.1789E-05	8.83472E+00
			30.00	7.54	4.22686E-05	4.5542E+00
			40.00	8.6	6.31803E-05	3.04684E+00
			50.00	9.76	8.1423E-05	2.3642E+00
			60.00	11.79	9.57771E-05	2.00988E+00
			60.09	11.99	9.58733E-05	2.00786E+00
			60.00	12.19	9.57771E-05	2.00988E+00
			50.00	14.22	8.1423E-05	2.3642E+00
			40.00	15.38	6.31803E-05	3.04684E+00
			30.00	16.44	4.22686E-05	4.5542E+00
			20.00	17.47	2.1789E-05	8.83472E+00
			10.00	18.54	6.88953E-06	2.79409E+01
			5.00	19.1	2.99376E-06	6.43003E+01
			0.00	19.79	0E+00	Infinity
		Depth (cm) = 1.000E-003				
		Depth Point (cm) = None				
		Average Rate Constant (sec**-1) = 5.06E-05				
		Integrated Rate Constant (day**-1) = 2.84E+00				
		Integrated Half-Life (days) = 2.44E-01				
50	WINTER		0.00	7.72	0E+00	Infinity
			5.00	8.46	2.9516E-06	6.52189E+01
			10.00	9.19	6.7859E-06	2.83677E+01
			19.86	12.08	2.12528E-05	9.05763E+00
			10.00	14.98	6.7859E-06	2.83677E+01
			5.00	15.7	2.9516E-06	6.52189E+01
			0.00	16.44	0E+00	Infinity
		Depth (cm) = 1.000E-003				

Latitude	Season	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
		Depth Point (cm) = None				
		Average Rate Constant (sec**-1) = 1.11E-05				
		Integrated Rate Constant (day**-1) = 3.48E-01				
		Integrated Half-Life (days) = 1.99E+00				

22. Under "Select Multiple Plots Case"
    a. Select **Selected Depth and Season vs Latitudes**
    b. Click Plot Multiple Rate Constants. The results are shown in Figure 17. *Note: the colors for the plot lines are chosen randomly by the program and will be different each time a plot is generated.*

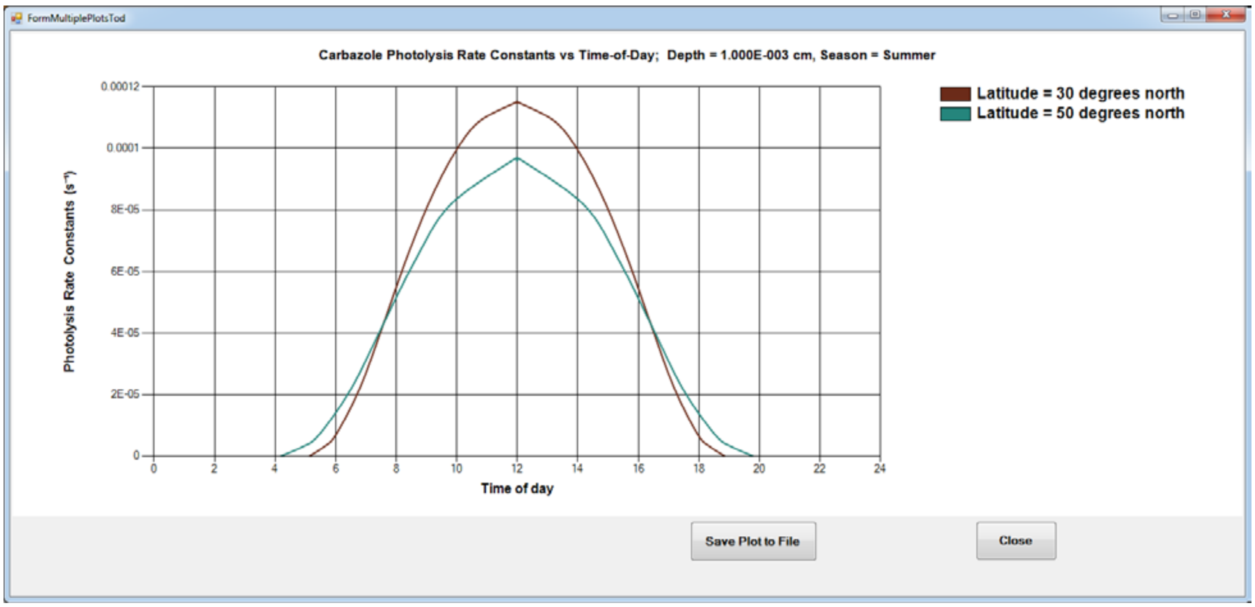

Figure 17. *The Multiple Plots tool showing multiple latitudes with the changes made during Part III of this walkthrough.*

23. Close the plot window.
24. Close the output window

3.4 PART IV: Non-default Ephemeride and Ozone Values

25. From the Modify Values module, under "Would you like typical ephemeride values?"
    a. Set **Would you like typical ephemeride values?** to: No. See Figure 18 for settings for Part IV.

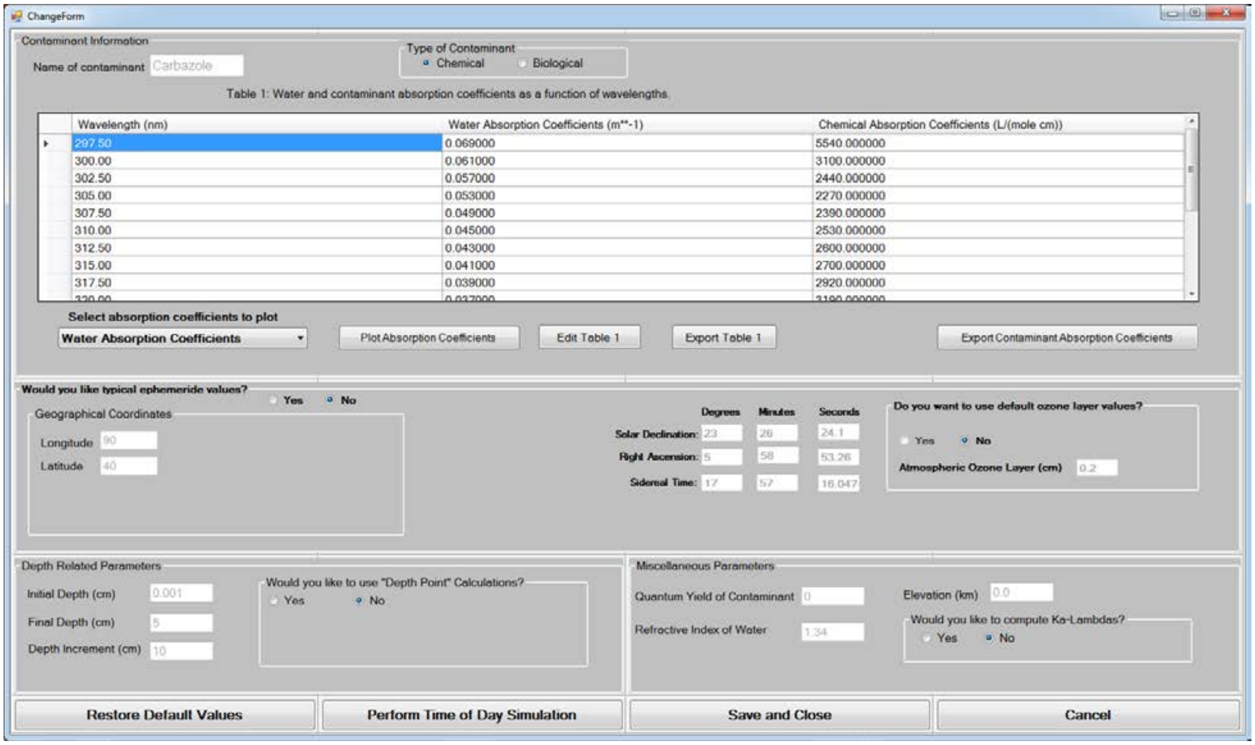

Figure 18. *The Modify Values module shown with "No" selected for typical ephemeride values. Note the change in what input fields are available under ephemeride values section.*

b. Under "Geographical Coordinates"
   i. Set **Longitude**: 83.2
   ii. Set **Latitude**: 34
c. Set **Solar Declination** to: 23 Degrees, 26 Minutes, 24.1 Seconds
d. Set **Right Ascension** to: 5 Degrees, 58 Minutes, 53.26 Seconds
e. Set **Sidereal Time** to: 17 Degrees, 57 Minutes, 16.047 Seconds
f. Under "Do you want to use default ozone layer values?"
   i. Set **Do you want to use default ozone layer values?** to: No
   ii. Set **Atmospheric Ozone Layer (cm)**: 0.200

26. Click Perform Time of Day Simulation

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	3.28244E-06	5.86454E+01
		10.00	5.24	7.59776E-06	2.53364E+01
		20.00	6.09	2.40599E-05	8.00086E+00
		30.00	6.91	4.64846E-05	4.14116E+00
		40.00	7.72	6.9212E-05	2.78131E+00
		50.00	8.52	8.89404E-05	2.16437E+00
		60.00	9.33	1.04411E-04	1.84367E+00

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
		70.00	10.18	1.15354E-04	1.66878E+00
		79.44	11.47	1.21476E-04	1.58468E+00
		70.00	12.76	1.15354E-04	1.66878E+00
		60.00	13.61	1.04411E-04	1.84367E+00
		50.00	14.42	8.89404E-05	2.16437E+00
		40.00	15.23	6.9212E-05	2.78131E+00
		30.00	16.03	4.64846E-05	4.14116E+00
		20.00	16.85	2.40599E-05	8.00086E+00
		10.00	17.7	7.59776E-06	2.53364E+01
		5.00	18.14	3.28244E-06	5.86454E+01
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 1.000E-003				
	Depth Point (cm) = None				
	Average Rate Constant (sec**-1) = 6.7E-05				
	Integrated Rate Constant (day**-1) = 3.47E+00				
	Integrated Half-Life (days) = 2E-01				

27. Close the output window

3.5 PART V: Changing Depth Parameters

28. From the Modify Values module, under "Depth Related Parameters"
    a. Set **Initial Depth (cm)**: 0.001 *(default)*
    b. Set **Final Depth (cm)**: 4000.001
    c. Set **Depth Increment (cm)**: 1000
29. Click Perform Time of Day Simulation

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	3.28244E-06	5.86454E+01
		10.00	5.24	7.59776E-06	2.53364E+01
		20.00	6.09	2.40599E-05	8.00086E+00
		30.00	6.91	4.64846E-05	4.14116E+00
		40.00	7.72	6.9212E-05	2.78131E+00
		50.00	8.52	8.89404E-05	2.16437E+00
		60.00	9.33	1.04411E-04	1.84367E+00
		70.00	10.18	1.15354E-04	1.66878E+00
		79.44	11.47	1.21476E-04	1.58468E+00
		70.00	12.76	1.15354E-04	1.66878E+00
		60.00	13.61	1.04411E-04	1.84367E+00

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
		50.00	14.42	8.89404E-05	2.16437E+00
		40.00	15.23	6.9212E-05	2.78131E+00
		30.00	16.03	4.64846E-05	4.14116E+00
		20.00	16.85	2.40599E-05	8.00086E+00
		10.00	17.7	7.59776E-06	2.53364E+01
		5.00	18.14	3.28244E-06	5.86454E+01
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 1.000E-003				
	Depth Point (cm) = None				
	Average Rate Constant (sec**-1) = 6.7E-05				
	Integrated Rate Constant (day**-1) = 3.47E+00				
	Integrated Half-Life (days) = 2E-01				
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	2.29243E-06	8.39721E+01
		10.00	5.24	5.25182E-06	3.66539E+01
		20.00	6.09	1.62903E-05	1.18168E+01
		30.00	6.91	3.12126E-05	6.16739E+00
		40.00	7.72	4.65739E-05	4.13322E+00
		50.00	8.52	6.02411E-05	3.19549E+00
		60.00	9.33	7.12233E-05	2.70277E+00
		70.00	10.18	7.91462E-05	2.43221E+00
		79.44	11.47	8.36391E-05	2.30156E+00
		70.00	12.76	7.91462E-05	2.43221E+00
		60.00	13.61	7.12233E-05	2.70277E+00
		50.00	14.42	6.02411E-05	3.19549E+00
		40.00	15.23	4.65739E-05	4.13322E+00
		30.00	16.03	3.12126E-05	6.16739E+00
		20.00	16.85	1.62903E-05	1.18168E+01
		10.00	17.7	5.25182E-06	3.66539E+01
		5.00	18.14	2.29243E-06	8.39721E+01
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 1.000E+003				
	Depth Point (cm) = None				
	Average Rate Constant (sec**-1) = 4.57E-05				
	Integrated Rate Constant (day**-1) = 2.36E+00				
	Integrated Half-Life (days) = 2.93E-01				
34		0.00	4.28	0E+00	Infinity

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
		5.00	4.81	1.68619E-06	1.14163E+02
		10.00	5.24	3.83592E-06	5.01836E+01
		20.00	6.09	1.17385E-05	1.63991E+01
		30.00	6.91	2.23739E-05	8.60379E+00
		40.00	7.72	3.34479E-05	5.75522E+00
		50.00	8.52	4.34797E-05	4.42735E+00
		60.00	9.33	5.1688E-05	3.72427E+00
		70.00	10.18	5.76987E-05	3.3363E+00
		79.44	11.47	6.11428E-05	3.14837E+00
		70.00	12.76	5.76987E-05	3.3363E+00
		60.00	13.61	5.1688E-05	3.72427E+00
		50.00	14.42	4.34797E-05	4.42735E+00
		40.00	15.23	3.34479E-05	5.75522E+00
		30.00	16.03	2.23739E-05	8.60379E+00
		20.00	16.85	1.17385E-05	1.63991E+01
		10.00	17.7	3.83592E-06	5.01836E+01
		5.00	18.14	1.68619E-06	1.14163E+02
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 2.000E+003				
	Depth Point (cm) = None				
	Average Rate Constant (sec**-1) = 3.31E-05				
	Integrated Rate Constant (day**-1) = 1.71E+00				
	Integrated Half-Life (days) = 4.04E-01				
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	1.29751E-06	1.48361E+02
		10.00	5.24	2.93806E-06	6.55195E+01
		20.00	6.09	8.91451E-06	2.1594E+01
		30.00	6.91	1.69373E-05	1.13655E+01
		40.00	7.72	2.53558E-05	7.59195E+00
		50.00	8.52	3.30768E-05	5.81979E+00
		60.00	9.33	3.94751E-05	4.87649E+00
		70.00	10.18	4.4211E-05	4.35412E+00
		79.44	11.47	4.69452E-05	4.10052E+00
		70.00	12.76	4.4211E-05	4.35412E+00
		60.00	13.61	3.94751E-05	4.87649E+00
		50.00	14.42	3.30768E-05	5.81979E+00
		40.00	15.23	2.53558E-05	7.59195E+00
		30.00	16.03	1.69373E-05	1.13655E+01

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
		20.00	16.85	8.91451E-06	2.1594E+01
		10.00	17.7	2.93806E-06	6.55195E+01
		5.00	18.14	1.29751E-06	1.48361E+02
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 3.000E+003				
	Depth Point (cm) = None				
	Average Rate Constant (sec**-1) = 2.53E-05				
	Integrated Rate Constant (day**-1) = 1.31E+00				
	Integrated Half-Life (days) = 5.3E-01				
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	1.03719E-06	1.85598E+02
		10.00	5.24	2.34158E-06	8.22094E+01
		20.00	6.09	7.06765E-06	2.72368E+01
		30.00	6.91	1.34028E-05	1.43626E+01
		40.00	7.72	2.00835E-05	9.58499E+00
		50.00	8.52	2.62604E-05	7.33043E+00
		60.00	9.33	3.14234E-05	6.12601E+00
		70.00	10.18	3.52734E-05	5.45737E+00
		79.44	11.47	3.7508E-05	5.13224E+00
		70.00	12.76	3.52734E-05	5.45737E+00
		60.00	13.61	3.14234E-05	6.12601E+00
		50.00	14.42	2.62604E-05	7.33043E+00
		40.00	15.23	2.00835E-05	9.58499E+00
		30.00	16.03	1.34028E-05	1.43626E+01
		20.00	16.85	7.06765E-06	2.72368E+01
		10.00	17.7	2.34158E-06	8.22094E+01
		5.00	18.14	1.03719E-06	1.85598E+02
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 4.000E+003				
	Depth Point (cm) = None				
	Average Rate Constant (sec**-1) = 2.01E-05				
	Integrated Rate Constant (day**-1) = 1.04E+00				
	Integrated Half-Life (days) = 6.65E-01				

30. Under "Select Multiple Plots Case"
    a. Select **Selected Latitude and Season vs Depths**
    b. Click Plot Multiple Rate Constants. The results are shown in Figure 19. *Note:*

the colors for the plot lines are chosen randomly by the program and will be different each time a plot is generated.

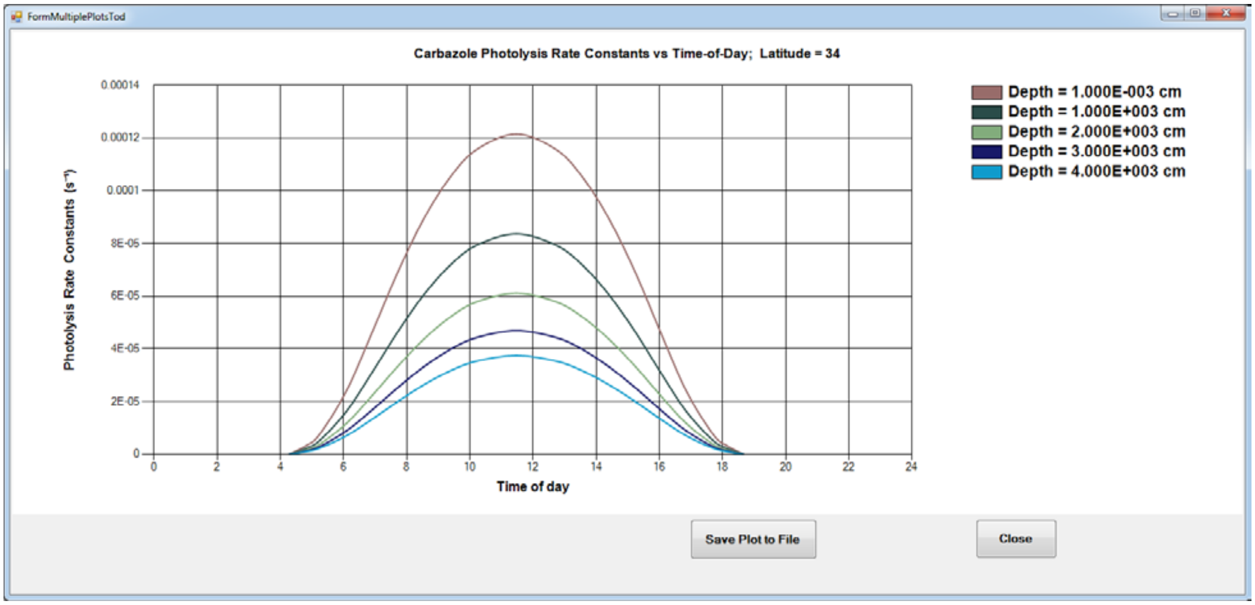

Figure 19. *The Multiple Plots tool showing multiple depths with the changes made during Part V of this walkthrough.*

31. Close the plot window
32. Close the output window

3.6 PART VI: Changing Depth Point

33. From the Modify Values module, under "Depth Related Parameters"
    c. Under "Would you like to use "Depth Point" Calculations?"
        i. Select "Yes"
        ii. Set **Depth Point (cm)**: 0.001 *(default)*
34. Click Perform Time of Day Simulation

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	3.28244E-06	5.86454E+01
		10.00	5.24	7.59775E-06	2.53364E+01
		20.00	6.09	2.40599E-05	8.00087E+00
		30.00	6.91	4.64845E-05	4.14116E+00
		40.00	7.72	6.92119E-05	2.78131E+00
		50.00	8.52	8.89404E-05	2.16437E+00
		60.00	9.33	1.04411E-04	1.84367E+00
		70.00	10.18	1.15354E-04	1.66878E+00
		79.44	11.47	1.21476E-04	1.58468E+00
		70.00	12.76	1.15354E-04	1.66878E+00

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
		60.00	13.61	1.04411E-04	1.84367E+00
		50.00	14.42	8.89404E-05	2.16437E+00
		40.00	15.23	6.92119E-05	2.78131E+00
		30.00	16.03	4.64845E-05	4.14116E+00
		20.00	16.85	2.40599E-05	8.00087E+00
		10.00	17.7	7.59775E-06	2.53364E+01
		5.00	18.14	3.28244E-06	5.86454E+01
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 1.000E-003				
	Depth Point (cm) = 1E-03				
	Average Rate Constant (sec**-1) = 6.7E-05				
	Integrated Rate Constant (day**-1) = 3.47E+00				
	Integrated Half-Life (days) = 2E-01				
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	1.53132E-06	1.25708E+02
		10.00	5.24	3.46349E-06	5.55798E+01
		20.00	6.09	1.04708E-05	1.83845E+01
		30.00	6.91	1.98571E-05	9.69429E+00
		40.00	7.72	2.97267E-05	6.47565E+00
		50.00	8.52	3.87983E-05	4.96156E+00
		60.00	9.33	4.632E-05	4.15587E+00
		70.00	10.18	5.18834E-05	3.71024E+00
		79.44	11.47	5.50919E-05	3.49416E+00
		70.00	12.76	5.18834E-05	3.71024E+00
		60.00	13.61	4.632E-05	4.15587E+00
		50.00	14.42	3.87983E-05	4.96156E+00
		40.00	15.23	2.97267E-05	6.47565E+00
		30.00	16.03	1.98571E-05	9.69429E+00
		20.00	16.85	1.04708E-05	1.83845E+01
		10.00	17.7	3.46349E-06	5.55798E+01
		5.00	18.14	1.53132E-06	1.25708E+02
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 1.000E+003				
	Depth Point (cm) = 1E-03				
	Average Rate Constant (sec**-1) = 2.97E-05				
	Integrated Rate Constant (day**-1) = 1.54E+00				
	Integrated Half-Life (days) = 4.51E-01				

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	7.30424E-07	2.63545E+02
		10.00	5.24	1.61798E-06	1.18976E+02
		20.00	6.09	4.69985E-06	4.09588E+01
		30.00	6.91	8.77657E-06	2.19334E+01
		40.00	7.72	1.32305E-05	1.45497E+01
		50.00	8.52	1.75653E-05	1.09591E+01
		60.00	9.33	2.13618E-05	9.01141E+00
		70.00	10.18	2.42944E-05	7.92364E+00
		79.44	11.47	2.60358E-05	7.39367E+00
		70.00	12.76	2.42944E-05	7.92364E+00
		60.00	13.61	2.13618E-05	9.01141E+00
		50.00	14.42	1.75653E-05	1.09591E+01
		40.00	15.23	1.32305E-05	1.45497E+01
		30.00	16.03	8.77657E-06	2.19334E+01
		20.00	16.85	4.69985E-06	4.09588E+01
		10.00	17.7	1.61798E-06	1.18976E+02
		5.00	18.14	7.30424E-07	2.63545E+02
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 2.000E+003				
	Depth Point (cm) = 1E-03				
	Average Rate Constant (sec**-1) = 1.37E-05				
	Integrated Rate Constant (day**-1) = 7.07E-01				
	Integrated Half-Life (days) = 9.81E-01				
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	3.56204E-07	5.4042E+02
		10.00	5.24	7.73954E-07	2.48723E+02
		20.00	6.09	2.17079E-06	8.86774E+01
		30.00	6.91	4.00046E-06	4.81194E+01
		40.00	7.72	6.07654E-06	3.16792E+01
		50.00	8.52	8.21196E-06	2.34414E+01
		60.00	9.33	1.01821E-05	1.89057E+01
		70.00	10.18	1.17672E-05	1.63591E+01
		79.44	11.47	1.27343E-05	1.51167E+01
		70.00	12.76	1.17672E-05	1.63591E+01
		60.00	13.61	1.01821E-05	1.89057E+01
		50.00	14.42	8.21196E-06	2.34414E+01
		40.00	15.23	6.07654E-06	3.16792E+01

Latitude	Summary Items	Solar Altitude	Time of Day (hours)	Rate Constant (sec**-1)	Half-Life (hours)
		30.00	16.03	4.00046E-06	4.81194E+01
		20.00	16.85	2.17079E-06	8.86774E+01
		10.00	17.7	7.73954E-07	2.48723E+02
		5.00	18.14	3.56204E-07	5.4042E+02
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 3.000E+003				
	Depth Point (cm) = 1E-03				
	Average Rate Constant (sec**-1) = 6.49E-06				
	Integrated Rate Constant (day**-1) = 3.36E-01				
	Integrated Half-Life (days) = 2.06E+00				
34		0.00	4.28	0E+00	Infinity
		5.00	4.81	1.77739E-07	1.08305E+03
		10.00	5.24	3.79115E-07	5.07762E+02
		20.00	6.09	1.03053E-06	1.86797E+02
		30.00	6.91	1.8769E-06	1.02563E+02
		40.00	7.72	2.87268E-06	6.70105E+01
		50.00	8.52	3.95197E-06	4.87099E+01
		60.00	9.33	4.9974E-06	3.852E+01
		70.00	10.18	5.87078E-06	3.27895E+01
		79.44	11.47	6.4172E-06	2.99975E+01
		70.00	12.76	5.87078E-06	3.27895E+01
		60.00	13.61	4.9974E-06	3.852E+01
		50.00	14.42	3.95197E-06	4.87099E+01
		40.00	15.23	2.87268E-06	6.70105E+01
		30.00	16.03	1.8769E-06	1.02563E+02
		20.00	16.85	1.03053E-06	1.86797E+02
		10.00	17.7	3.79115E-07	5.07762E+02
		5.00	18.14	1.77739E-07	1.08305E+03
		0.00	18.66	0E+00	Infinity
	Depth (cm) = 4.000E+003				
	Depth Point (cm) = 1E-03				
	Average Rate Constant (sec**-1) = 3.18E-06				
	Integrated Rate Constant (day**-1) = 1.65E-01				
	Integrated Half-Life (days) = 4.2E+00				

This ends the sample session.

Appendix I: Default Values

Contaminant Name: Methoxyclor

Initial Depth: 0.001 cm

Quantum Yield: 0.32

Water identification: Pure Water

Depth Increment: 10 cm

Seasons: Spring

Type of atmosphere: Terrestrial

Final Depth: 5 cm

Latitude: 34

Longitude: 83.2

Depth Point: 0.0

Elevation: 0 km

Refractive Index: 1.34

Wavelength (nm)	**Water Absorption Coefficients (m**-1)**	**Chemical Absorption Coefficients (L/(mole cm))**
280.00	0.120000	2200.000000
282.50	0.113000	2020.000000
285.00	0.106000	1530.000000
287.50	0.099000	642.000000
290.00	0.093000	271.000000
292.50	0.085000	102.000000
295.00	0.077000	28.000000
297.50	0.069000	11.100000
300.00	0.061000	4.670000
302.50	0.057000	1.900000
305.00	0.053000	1.100000
307.50	0.049000	0.800000
310.00	0.045000	0.530000
312.50	0.043000	0.330000
315.00	0.041000	0.270000
317.50	0.039000	0.160000
320.00	0.037000	0.100000
323.10	0.035000	0.060000
330.00	0.029000	0.020000
340.00	0.024000	0.000000
350.00	0.020000	0.000000
360.00	0.016000	0.000000
370.00	0.013000	0.000000
380.00	0.009600	0.000000
390.00	0.008300	0.000000
400.00	0.007400	0.000000
410.00	0.007000	0.000000
420.00	0.006600	0.000000
430.00	0.006200	0.000000

Wavelength (nm)	Water Absorption Coefficients (m**-1)	Chemical Absorption Coefficients (L/(mole cm))
440.00	0.006200	0.000000
450.00	0.006200	0.000000
460.00	0.006800	0.000000
470.00	0.006800	0.000000
480.00	0.007600	0.000000
490.00	0.008500	0.000000
500.00	0.012000	0.000000
525.00	0.021000	0.000000
550.00	0.028000	0.000000
575.00	0.041000	0.000000
600.00	0.100000	0.000000
625.00	0.140000	0.000000
650.00	0.150000	0.000000
675.00	0.190000	0.000000
700.00	0.280000	0.000000
750.00	1.000000	0.000000
800.00	0.890000	0.000000

The table below contains the default ozone layer's thicknesses used in GCSolar. There is an ozone layer thickness for each of the 10 latitudes and 4 seasons listed below, for a total of 40 values. Ozone layer data are in cm and latitudes are in degrees.

Latitude	Spring	Summer	Fall	Winter
0	0.26	0.256	0.244	0.241
10	0.268	0.261	0.253	0.247
20	0.287	0.273	0.261	0.26
30	0.313	0.292	0.27	0.284
40	0.352	0.314	0.281	0.318
50	0.395	0.333	0.299	0.357
60	0.419	0.346	0.308	0.373
70	0.43	0.349	0.307	0.37
80	0.435	0.347	0.299	0.364
90	0.436	0.339	0.29	0.361