

Vis I I 05 SPECTROPHOTOMETER SOFTWARE USER'S MANUAL

Version 1.1E

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Introduction

The UNICO® Application Software—VIS-I 105 has been designed to operate with UNICO® Spectrophotometer Model Vis-I 105. The software runs on a PC (personal computer) with Windows® 95/98/Me/NT/2000/XP operating system installed.

Your **UNICO**[®] **Application Software** package includes:

- One CD containing the software (**VIS-I 105**)
- Software User's Manual
- A 6' null modem connection cable with 9-pin female connector's on both ends.

The UNICO® Application Software performs the following methods for analysis:

Absorbance/%Transmittance/Concentration: measure the Absorbance, %Transmittance, Concentration/Standard, or Concentration/Factor at a single wavelength within the range of **340**~**1000** nm.

Standard Curve: create a calibration curve (choice of 4 curve fits) with up to 8 standard solutions at a single wavelength to determine concentrations of unknown samples.

Kinetics (Absorbance vs. Time Kinetics): measure a sample's absorbance change over a selected period of time, store the test results in data table, display the results graphically, and calculate the reaction rate within a given time interval.

Minimum Computer Requirements

To properly install and operate the enclosed software, it is required to have the following minimum computer configuration:

PC with:

- I6MB RAM
- Pentium or faster processor
- 10 MB of free space on memory
- VGA Color Monitor
- PS/2 mouse and keyboard

NOTE: The **UNICO® Application Software** provided will **NOT** function with a **Macintosh/Apple** or **Linux** computer.

Software Installation

Loading Software to Computer

To install the software, please close any open programs and disconnect from the Internet if online, then follow the instructions below.

- Step I: Insert **UNICO® Application Software** CD into the CD drive of your **PC.**Go to **Start,Run** and type F:\setup. Welcome to the Vis-I I 05 Spectromenter setup program refer fo Figure-I
- Step 2: Enter personal details such as Company Name and User Name
- Step 3: Provide program Installation path as shown in Figure 3:
- Step 4: Commence the installation of the Vis-1105 program
- Step 5: Complete the Installation Process of the Vis-1105 Program

NOTE: If you wish to change the location of the installation, then click Change Directory and specify the desired directory. If you are unsure and need to examine your computer files, click on Exit Setup and go to Windows. Explorer to make sure no duplication or improper storage of the files will occur.

Congratulations! You have now installed your **UNICO**® **Application Software** VIS-II05 in your PC for your VIS-II05 Spectrophotometer.

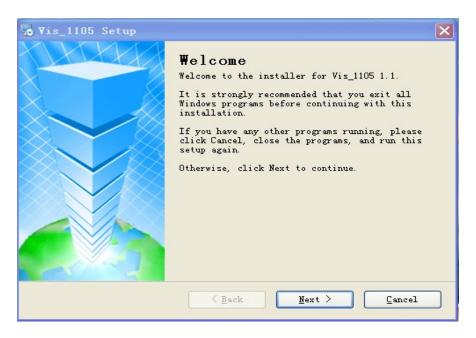


Figure-1: Welcome to the Vis-1105 Spectrometer Setup Procedure

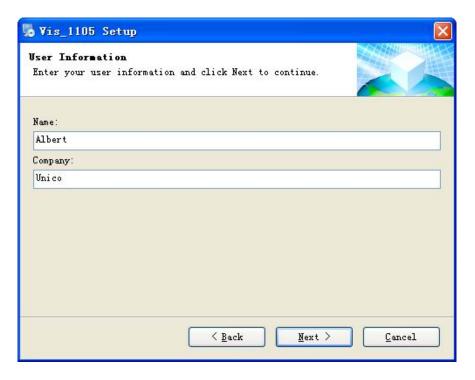


Figure-2: Enter personal details Name and Company

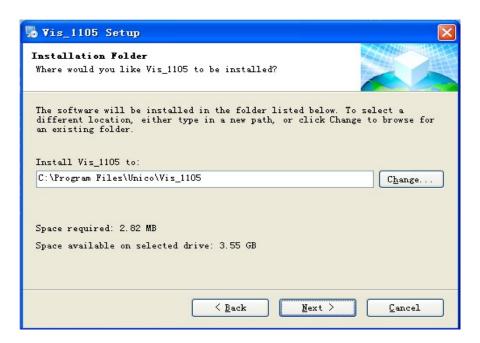


Figure-3 Program directory path for installation recommended

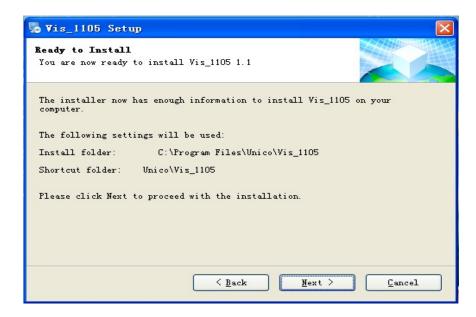


Figure-4 Commence Installation of the Vis-1105 Software



Figure-5 Installation Successful

Connecting Computer to Spectrophotometer

- Step 1: Remove the RS232 Connection Cable (double end) out of the bag.
- Step 2: Locate the RS-232C port on the back of your PC. Connect the female 9-pin (small) connector (one end of the Connection Cable) to the male 9-pin of your PC and secure with the built-in screws.
- Step 3: **Vis-1105** Spectrophotometer has a male 9-pin RS-232C port on the back panel, located to the left side of the **Vis-1105**. Connect the other end of the connection cable to your **Vis-1105** and secure it tightly.
- Step 4: Turn on your PC (if not already on) and your **Vis-I I 05** (if not already on and let it warm up for fifteen minutes).
- Step 5: Click the **Start** button on your PC, scroll to **Programs**, **UNICO**® **Application Software** and locate the **Vis-I 105** (Figure-I 0), and click it.
- Step 6: The Start-up Screen of **Vis-II05** will appear as Figure-II shown.
- Step 7: Select the proper port, and then click **OK** on your Computer Screen. The **Vis-1105** will initialize and go to the main screen (Figure-12).

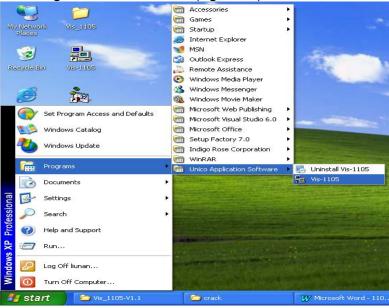


Figure-10 Open the Software



Figure-11 Start-up Screen

Main Screen Display

After your **Vis-1105** is connected to your PC, and **Vis-1105** is running, your PC will show the **Main Screen Display** like Figure-12. Type your **User Name** in the Text Field at the right of the **User Name** (<u>U</u>): label or leave it blank, then click the **OK** button to login as Figure-13 shown.

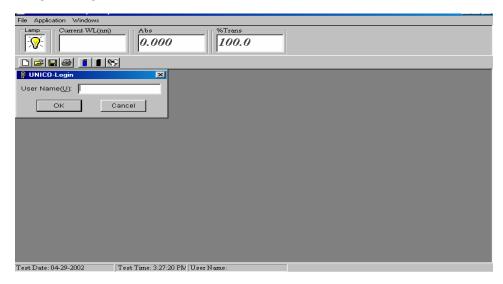


Figure-12 Main Screen Display



Figure-13 Main Screen Display After User Login

Functions of Drop-down Menu, Text Field, and Icon Button

Drop-down Menu

Two **Drop-down Menus**: **File** (Figure-14) and **Application** (Figure-15) are illustrated below.



Figure-14 File Drop-down Menu

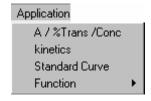


Figure-15 Application Drop-down Menu

File Drop-down Menu has six functions: New User, New, Load, Save as, Print, and Exit. All of them have hot keys except the first one.

- New User: change user name
- New: reset Text Parameter and begin new test
- Load: open any saved file (.tst)

- Save as: save the setup or data displayed
- **Print**: print all information shown in the Data Screen and any data collected.
- Exit: quit the Vis-I 105

Application Drop-down Menu can select three Analytical Methods of the Vis-I 105 Spectrophotometer: A/%Trans/Conc, Kinetics, and Standard Curve.

- A/%Trans/Conc: measure Absorbance, %Transmittance, Concentration/Standard, or Concentration/Factor.
- **Kinetics**: measure a sample's **Absorbance** change over a selected period of time, store the test results in data table, display the results graphically, and calculate the reaction rate within a given time interval (**Function Menu** is part of the **Kinetics Analytical Method**).
- **Standard Curve**: create a calibration curve (choice of 4 curve fits) with up to 8 standard solutions to determine **Concentrations** of unknown samples.

Text Field

Three Text Fields are just below **File Drop-down Menu** and under the label: **Current WL(nm)**, **Abs**, and **%Trans** (Figure-16).



Figure-16 Text Field

Current WL(nm) Text Field: display the last selected wavelength of the spectrophotometer (manually entered).

Abs Text Field: display the current data in Absorbance.

%Trans Text Field: display the current data in %Transmittance.

Icon Button

Seven **Icon Buttons** are below the Text Field (Figure-17).



Figure-17 **Icon Button**

The four Icon Buttons counting from the left end of the Figure-17 have the same functions as **New**, **Load**, **Save as**, **Print** of the **File Drop-down Menu**.

OA/100%T Icon Button: set **O Absorbance** and **100%T**. Insert reference into **Sample Compartment** and click button (blue colored) (move cursor on to the blue cuvette icon--the fifth icon from left end of Figure-17 and right touch the mouse, it will show **OA/100%T** sign) (Figure-18).



Figure-18 **0A/I00%T Icon Button** for **BLANKING**

0%T Icon Button: set **0%T**. Click button (black colored) (move cursor on to the black cuvette icon--the sixth icon from left end of Figure-17 and right touch the mouse, it will show **0%T** sign) (Figure-19).



Figure-19 **0%T Icon Button**

Reset Button: unlock the screen. If the screen frozen due to improper operations, **BLANK** may show in the Text Fields below **Abs** and %**Trans** labels (Figure-16), click button to reset them and unlock the screen.

Basic Operation

IMPORTANT: Do not use the button on the spectrophotometer. Set 0%T and blank only from the software. (It is normal if the display on the spectrophotometer is slightly different from the display on PC screen).

Three Analytical Methods--Absorbance/%Transmittance/Concentration, Standard Curve, and Absorbance vs. Time Kinetics are illustrated below.

Absorbance, %Transmittance, Concentration

The Absorbance, %Transmittance, Concentration (A/%Trans/Conc) method has the following three modes of operation:

- Absorbance/%Transmittance
- Concentration/Standard
- Concentration/Factor

Main Screen of A/%Trans/Conc

At the Main Screen (Figure-13), click Application Drop-down Menu, and click A/%Trans/Conc (Figure-15) to enter the Main Screen of A/%Trans/Conc (Figure-20).

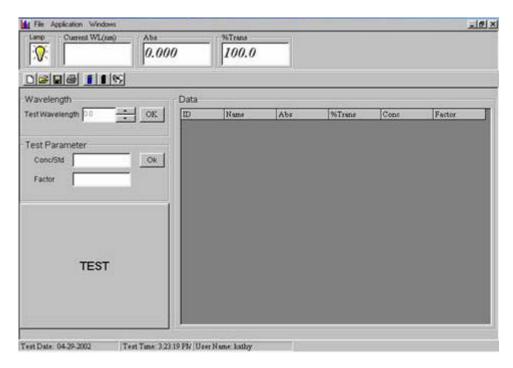


Figure-20 Main Screen of A/%Trans/Conc

The A/%Trans/Conc Analytical Method has five operation functions: Test Wavelength Text Field, Test Parameter Test Field, TEST Button, Data Table, and Test Date:

- on the spectrophotometer and clicking button on the PC screen, click **OK** button (Figure-21) at the right of button to set the wavelength (Figure-22). The wavelength will be shown both in the Text Field below **Current WL(nm)** label and Text Field at the right of the **Test Wavelength** label.
- Test Parameter Text Field: If standard solution is available, type the concentration values of the standard into the Text Field at the right of Conc/Std label, insert the standard into Sample Compartment and click the OK button. Spectrophotometer will take measurement of the standard and display factor value. The unknown sample concentrations can then be measured. If factor value is available, enter the factor value into the Text Field at the right of Factor label for the unknown sample concentrations calculation (Figure-21).
- **TEST** Button: record the readout of a given sample (Figure-23).
- Data Table: record ID, Name, Abs, %Trans, Conc, and Factor related with the test (Figure-23)
- **Test Date**: **Test Date** will be displayed automatically. To alter it, simply click it at the left corner of the screen and enter the desired date (Figure-24).

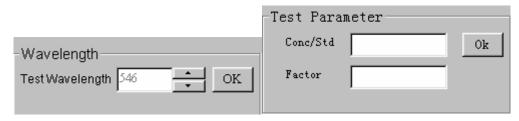


Figure-21 Test Wavelength and Test Parameter

Absorbance/%Transmittance Mode

The following are the basic operations (Figure-25).

- Step 1: Insert **reference** cuvette or nothing into the Sample Compartment and close the lid.
- Step 2: Select the desired wavelength by moving the WAVELENGTH dial on the Vis-
 - I 105. Click button on the PC screen to match the desired wavelength, click **OK** button at the right of button to set the wavelength.

DO NOT PUSH ANY BUTTONS ON THE Vis-1105. THIS MAY CAUSE FOR YOU TO RE-BOOT THE SOFTWARE.

- Step 4: Remove the reference (if it is there) and place your sample cuvette into the Sample Compartment, close the lid and click on **TEST** Button. The test results will be displayed in a spreadsheet format in the **Data Table**.
- Step5: You may type in sample name or change the sample name under the **Name** label inside the **Data Table**.

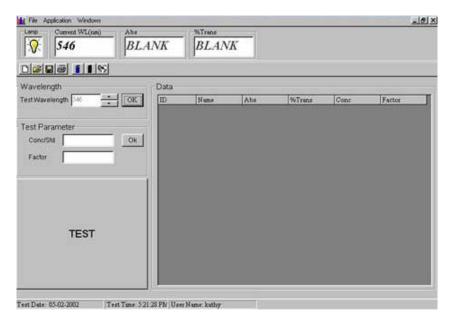


Figure-22 Wavelength and Reference Setting



Figure-23 **TEST** Button and **Data Table**

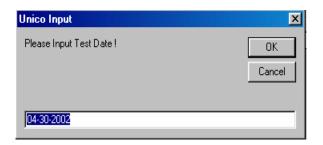


Figure-24 **Test Date**

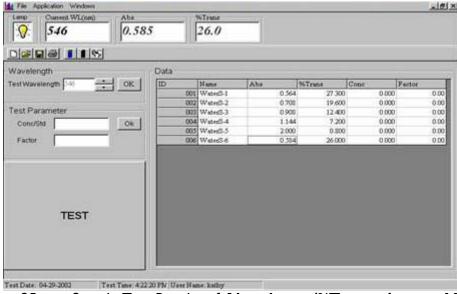


Figure-25 Sample Test Results of **Absorbance/%Transmittance Mode**

Concentration/Standard Mode

The purpose of this test is to determine the **Concentration** of the unknown samples by comparing the samples' **Absorbance/Transmittance** to that of the standard solution.

Repeat Step I to 3 in Absorbance/%Transmittance Mode section.

Step 4A: Type in the known concentration of the standard solution in the Text Field at the right of **Conc/Std** label.

Step 5A: Place the standard in the Sample Compartment and close the lid.

Step 6A: Click the **OK** Button in **Test Parameter** section. This will measure the **Absorbance** of the standard and set its conversion **Factor** for measuring the unknown samples (Figure-26).

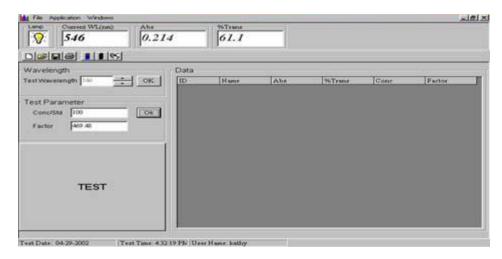


Figure-26 Standard Solution **Absorbance** Measurement

Step 7A: Place your sample(s) in the Sample Compartment and click the **TEST** Button for each sample to be measured. **Absorbance**, **Transmittance** and the **Concentration** of the samples will be displayed in the **Data Table** (Figure-27).

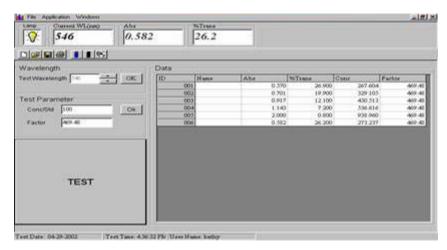


Figure-27 Sample Test Results of Concentration/Standard Mode

Concentration/Factor Mode

The purpose of this test is to measure the **Concentration** of the samples with known multiplication factor to calculate the **Concentration**.

Repeat Step I to 3 in Absorbance/%Transmittance Mode section.

Step 4B: Type in the desired **Factor** in the Text Field at the right of the **Factor** label.

Step 5B: For each sample, be sure to place the sample in Sample Compartment and close the lid. Click the **TEST** Button to record results. The **Absorbance**,

Transmittance and **Concentration** of the samples will be displayed in the **Data Table** (Figure-28).

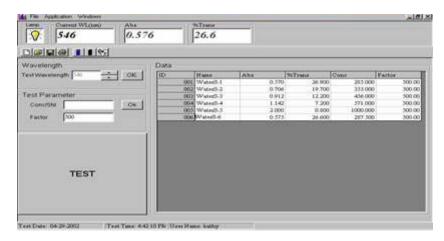


Figure-28 Sample Test Results of Concentration/Factor Mode

Standard Curve

The **Standard Curve** (Calibration Curve) method allows the operator to

- Measure up to 8 standards
- Calculate standard curves with 4 curve fits, including:
 - Linear Thru Zero: set the y-intercept equal to zero; therefore, the curve is forced through zero. Calculate and display the slope and Correlation Coefficient.
 - 2. **Linear Squares**: Linear regression model. Calculate and display the slope, y-intercept, and **Correlation Coefficient** for the given standards.
 - 3. **2nd Order**: second derivative of the **Linear Squares** model. Calculate and display the coefficients. This method is used for non-linear standard curves or curves with a **Correlation Coefficient** of less than 0.9.
 - 4. **Segmented**: straight line. Use the standards as nodes to connect each point. No data is displayed or calculated.
- Select and view existing standard curves
- Calculate the **Concentrations** of unknown samples

Main Screen of Standard Curve

At the Main Screen (Figure-13), click Application Drop-down Menu, and click Standard Curve (Figure-15) to enter the Main Screen of Standard Curve (Figure-29).

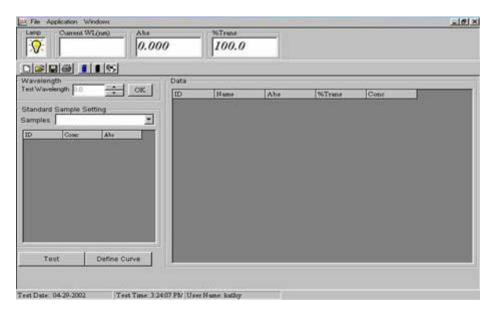


Figure-29 Standard Curve Setup

The following are the basic operations.

- Step 1: Insert reference cuvette or nothing into the Sample Compartment and close the lid.
- Step 2: Select the desired wavelength by moving the WAVELENGTH dial on the Vis-
 - 1105. Click button on the PC screen to match the desired wavelength, click OK button at the right of button to set the wavelength.
- Step 4: Under **Standard Sample Setting**, click the **Arrow** Button and set the number of standards (from 2 to 8) to be used (Figure-30).
- Step 5: Place the standards in the Sample Compartment in order of lowest concentration to highest concentration. Type the concentration of the standards (e.g. 0.14 here) into the Text Field starting below **Conc** label and at the right of **ID 01** as Figure-31 shown. Press **Enter** key on your computer keyboard or click with the mouse to move to the next cell. Repeat the same operation until all concentrations of the standards have been entered.
- Step 6: Measure the **Absorbance** of each standard. For each measurement, insert the standard into Sample Compartment and click **Test** button. The **Absorbance** and **Transmittance** values will be recorded into the **Data Table**; then, double click in the appropriate **Absorbance** cell (**Abs**) (in the left table) next to the standard **Conc** to get the **Absorbance** for curve drawing. Continue until all of the standards have been measured (Figure-31). Alternatively, if you do not want the **Absorbance** of the standards to be recorded into the **Data Table**, you may select the appropriate **Absorbance** cell (**Abs**) (in the left table) next to the standard **Conc** and double click the mouse to get the **Absorbance** results.
- Step 7: Press the **Define Curve** Button (Figure-31) to graph the **Standard Curve** (e.g. WaterS-1 to WaterS-6 are the standards) (Figure-32) and you may **save** it for future use.

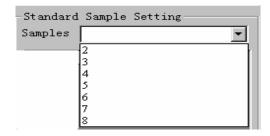


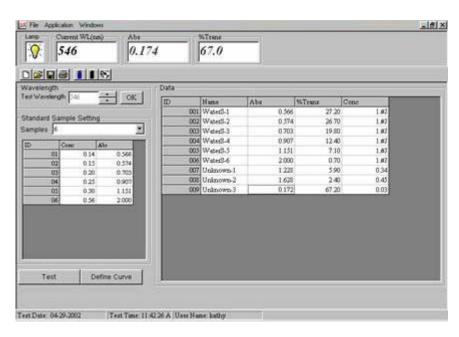
Figure-30 Standard Sample Setting

Your standards have now completed setup. To use the graph and measure the unknown sample concentrations, please be guided by the steps below:

Step 1: Select the desired **Standard Curve** by clicking on one of the four buttons (Figure-33). Shown in Figure-32 is **Linear Squares** (Least Squares Method). Items in the equation next to the **Linear Squares** title on the graph are Abs, the slope, and y-intercept as well as **Correlation Coefficient**

Abs = slope *C + y-intercept
Corr. Coef = Correlation Coefficient

- Step 2: (optional) Click **Print** button: print the graph and labels of the slope, y-intercept and Correlation Coefficient as seen on the screen.
- Step 3: When ready to measure samples of unknown concentration, press _____(arrow return button) to return to the main **Standard Curve** screen (Figure-31).
- Step 4: To measure the concentration of unknowns, place the samples in the Sample Compartment and click on **Test** button (Figure-31), located at the bottom-left portion of the screen.
- Step 5: To save the data with the **Standard Curve** fit selected, click on the (Save Icon), name the file, and click **Save**.



- 18 X %Trans 546 0.000 100.0 Linear square Linear This Zero Second Order Segmented Test Name Linear Square: Abs = 3.491964 * Conc + 0.052318 A 1=8 566 A 2×0.574 A 3=0.703 A 4=0.907 1.750 A 5=1.151 1.500 1,250 1.000 0.750 0.500 0.250 0.000 0.5 0.6 0.2 0.4 Test Date: 04-29-2002

Figure-31 Sample Test Results of **Standard Curve**

Figure-32 **Standard Curve** Graph Display



Figure-33 Buttons for **Standard Curve** Test

Kinetics

The **Kinetics** application has the following functions:

- Setup kinetics **Test Parameters**
- Obtain kinetics data for a sample at a single wavelength
- Load and save data files for further studies
- Get the reaction rate within a given time interval

Main Screen of Kinetics

At the **Main Screen** (Figure-13), click **Application Drop-down Menu**; click **Kinetics** (Figure-15) to enter the **Main Screen of Kinetics Test** (Figure 34).

The following are the basic operations.

Step 1: Insert **reference** cuvette or nothing into the Sample Compartment and close the lid. Step 2: Select the desired **wavelength** by moving the **WAVELENGTH** dial on the **Vis-**

1105. Click button on the PC screen to match the desired wavelength, click **OK** button at the right of button to set the wavelength.

Step 3: Click on **0A/I00%T Icon Button**—button (the blue cuvette icon) to **blank** the reference.

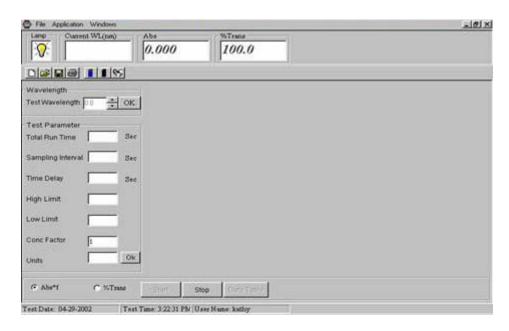


Figure-34 Kinetics Test Main Screen

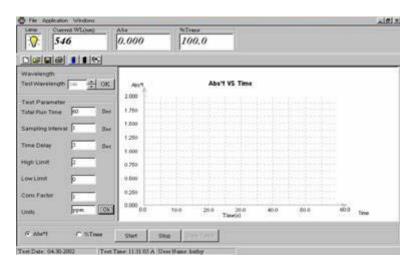


Figure-35 **Test Parameters** Setting

- Step 4: Set the **Test Parameters** (Figure-35) (**Step 4 to Step 8**). Set the **Total Run Time** by typing into the Text Field on the right of the **Total Run Time** label. This is the total time for the reaction to occur.
- Step 5: Set **Sampling Interval** time similar as **Step 4**. This is the time interval for which measurements will be recorded (i.e. every 10 s, or every 3 s, etc.).
- Step 6: Set an Initial **Time Delay** similar as **Step 4**. The purpose of this step is to delay the beginning of data collection. (i.e. Sample must be injected, and reaction will not begin for 20 s).

- Step 7: Set a **Conc Factor** (multiplication factor--dilution factor) similar as **Step 4**. This allows for a factor to be used when calculating the **Concentration** of the solution.
- Step 8: Set the **High** and **Low Limits** of the graph similar as **Step 4**. This is the selection of the minimum and maximum **Absorbance** range for the graph of the data.
- Step 9: Place your sample in the Sample Compartment and click the **Start** Button once all the **Test Parameters** have been set and you are ready to start your measurement (Figure-36).

Notes: **Data Table**: once measurements have been made, clicking this button will allow you to view the data collected (Figure-37). Only **Cell 2** of the **Data Table** is currently used to store the data collected, others are for future applications.

Stop Button: stops the data collection at any given moment.

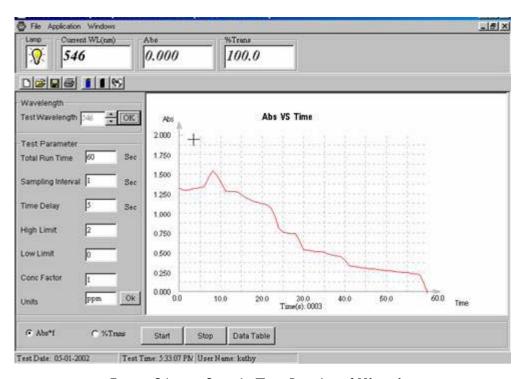


Figure-36 Sample Test Results of **Kinetics**

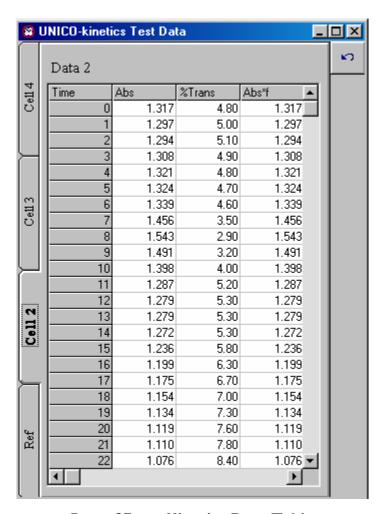


Figure-37 Kinetics Data Table

Math Function for Kinetics

Vis-1105 provides additional features for you to calculate the **reaction rate** within a given time interval.

After your Kinetic test, keep the test curve screen open.

- Click Application Drop-down Menu and click Function as Figure-38 shown.
- Click **K**, type the **start**, **end** time, and **factor** into the appropriate Text Fields in the pop up window as Figure-39 indicated. Press **confirm** button to get the **reaction rate** graph (Figure-40).

If you want to get another reaction rate for a different time interval, simply go to **Function**, click **Replace**, it will return to the original test curve screen; repeat the above mentioned procedure, you will get the new **reaction rate** graph.



Figure-38 Math Functions for Kinetics

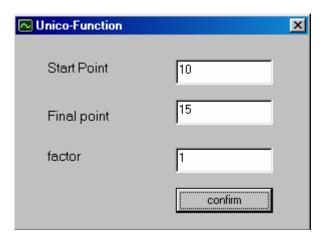


Figure-39 **Math Function** Setting

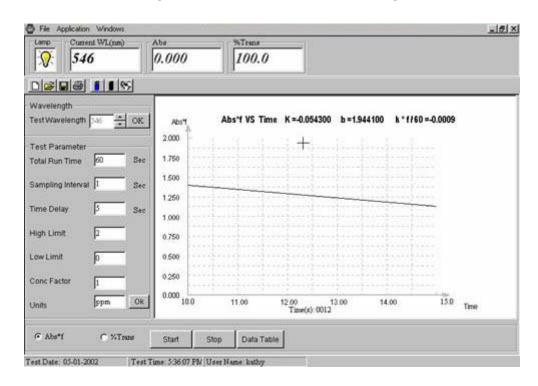


Figure-40 Sample Test Results of **Math Function of Kinetics**

Data import to Microsoft Excel®

By referring to the following steps, you can transfer any of the **UNICO® Application Software—Vis-I105** test data to a Microsoft Excel[®] program:

- Step 1: In Microsoft Excel, click on **File** and click **Open**.
- Step 2: Select any saved file you wish to import.
- Step 3: After the Excel Text Import Wizard appears, select **Delimited**, select the row from which you want the import to start, and click on the **Next** button as shown in Figure-41.
- Step 4: Uncheck the **Tab** delimiter and select **Comma** delimiter as shown in Figure-42, then click the **Next** button.
- Step 5: Click the **Finish** button and the test data will be imported into your Excel spreadsheet. Here, further calculations can be performed from the "raw" data collected.
- Step 6: Save the imported file under a DIFFERENT FILE Name if you still want to keep and open the original UNICO® data file in VISI-105. Otherwise, the original UNICO® data file (.tst file) will be modified by the Excel® format during importing and the modified file cannot be opened from VIS-1105.

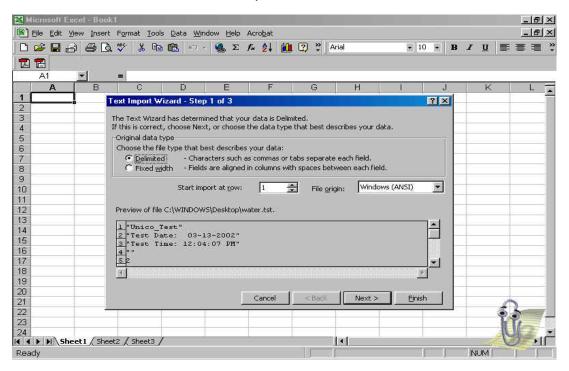


Figure-41 Excel Text Import Wizard I

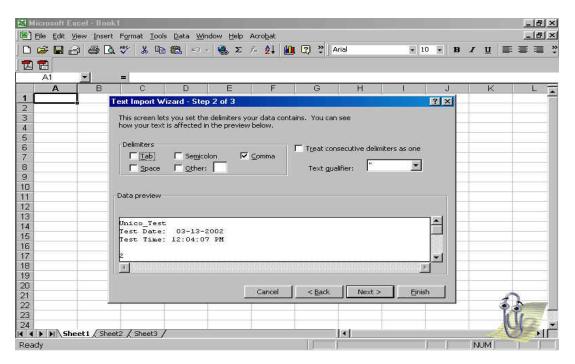


Figure-42 Excel Text Import Wizard II