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## **GETTING STARTED MANUAL**

### **POWERSUITE 2.40**

*Including:*

*Addendum for a quick startup and potentiostat CV test experiment*

#### **ATTENTION**

This manual is by no means a complete detailed operating manual of the PowerSuite software. It will serve as a better understanding of the startup and initial operations with this software, as well as the basic principles. This manual does not intend to give specifications or technique limitations. Fully detailed features are described in the html « help » section of the software.

## **SHORTFORM STARTUP MANUAL FOR POWERSUITE 2.40**

(MODULES [PowerSINE](#), [PowerCV](#), [PowerSTEP](#), [PowerPULSE](#), [PowerCORR](#))

This manual is only meant as a start-up guide and does not cover all features and details of the full software. For more detailed instructions and specifications, consult the help menu of your PowerSuite 2.40 software. It provides extended operating instructions in hypertext format. The help section is written in HTML format, for which your PC needs to be equipped with MS Explorer 4.0 as a minimum. This help section provides many application notes as well as theoretical basics and bibliographies.

This manual also has an addendum that covers an example for a quick test experiment. This allows you to quickly setup a CV measurement that will also serve to test that your potentiostat is operating properly.

**Special features that differentiate this software from any other product are:**

- **The database structure (Microsoft Access)**
- **Right mouse click operations**
- **Experiments are stored into database records, each including their proper setup, data and graph settings.**

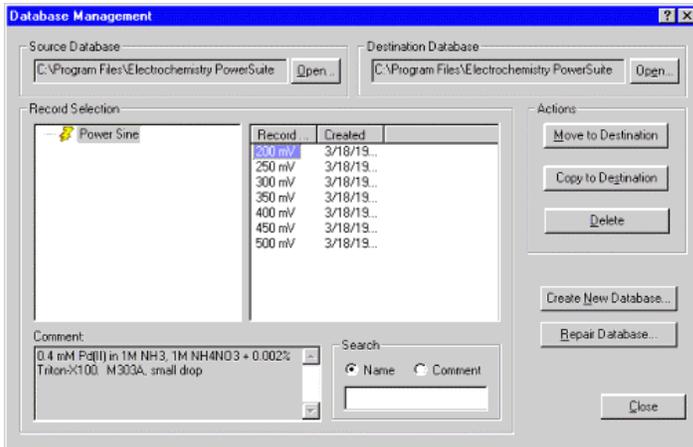
### **1) Connections to the potentiostat**

First, connect your potentiostat to the USB or GPIB interface and boot up. Follow the installation instructions for your PowerSuite module (PowerCV, PowerSTEP, PowerPULSE, PowerCORR or PowerSINE). Start up the software. In normal operation you should see the last data set recorded. Go to « **Experiment** » then « **Close** » to start from a blank page. Click on « **Tools** » then « **Search for Instruments** » in order to verify the communication with the potentiostat (The communication LEDs on the front panel of the potentiostat should blink at this moment. For the USB interfaced PARSTATS, after having installed the USB drivers from the installation CD-ROM, the LED named « COM » on the front panel will light up during this operation).

- ***Note:** With GPIB-controlled potentiostats making impedance measurements, a lock-in amplifier (FRD1025, 100, 2000 or 5210EC) or an FRA (1255 or 1260) will be connected to your potentiostat. The software (PowerSINE module) will first find the frequency analyzer and then request the type of potentiostat (click on the correct choice) being used.*

### **2) Database management system**

PowerSuite's data handling uses a database storage system, based on Microsoft Access. It does not operate with the classic DOS structured filing system. Each record in the database will store the data of an experiment, including all parameters and graph settings.



In this example, the source database contains PowerSINE experiments. There are 7 experiments, listed under the heading **Record**.

Upon first installation, PowerSuite creates a default database named « **Powerdata.mdb** ». Choosing « **Tools** », « **Database Management** » allows you to view the structure and location of this database. You can create a new database and allocate it to a specific user or research topic by choosing « **Create New Database** ». Thousands of records (experiments) can be recorded in one database.

- **Note:** You are not limited by the number of databases you can create.
- **Note:** The « **Powerdata.mdb** » database is the only database that will allow you to access the « **PowerStat** » function (a direct control function for the PARSTAT potentiostats), which is available via « **Experiment** », « **Open** ».

The **Record Selection** window shows the installed techniques (PowerCV, PowerSTEP, PowerPULSE, PowerCORR and/or PowerSINE) from the **Source Database**. The source database is the active database you are currently working in. On the right side of the **Record Selection** window, you will see the experimental data records from the selected technique. You can copy or move these data records from one database to another (selected in the **Destination Database** window) by using the commands « **Move to Destination** » or « **Copy to Destination** ».

- **Note:** You can copy your database to a different location on your computer. The path for your database location is indicated in the « **Source Database** » and « **Destination Database** » boxes.
- **Note:** Copying experimental data only and/or graphical data is performed in a different way (see section 9).

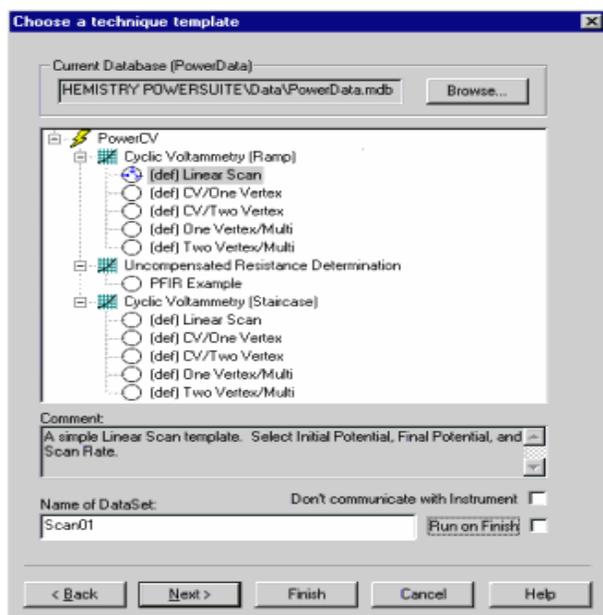
Databases allow you to search and select a record, or series of records, using keywords found in the comment field or name of a record. If you have previously entered comments in the **Comment** box of your experiment (found in the **Experimental Properties** setup), you can search those records for text matching the criteria entered into the **Search** box. The same can be done for the record names.

### 3) Creating an experimental setup

On the tool bar, when a blank page is active, you will find two icons, « **New** » and « **Open** ».

- « **New** » opens the New Experiment Wizard.
- « **Open** » opens an existing data set (or record) within the current database.

➤ ***Note:** These tools can also be found in the top banner under « **Experiment** ».*



To set up an experiment (or template), click on the « **New** » icon. The New Experiment Wizard will open up, then click on « **Next** ».

All the installed PowerSuite modules (yellow lightning icons), will now become listed. Open the module of your choice to view the templates installed by default.

**(PowerSuite has about 45 different techniques within the five modules available – version 2.40)**

#### 3-1: Choose a technique template Window

On the top of this page, you can choose the database into which you want to create and store your experiments. You can use « **Browse** » to view the different databases available. Double click on the installed module (or click once on the + sign), and the different techniques available (or previously created) will become listed. Double click on the technique of your choice (or click once on the + sign) to view the templates previously stored for this technique. If (def) is in front of them, they are default templates that can be used or modified. Once you have selected the template, a small blue pictogram will appear inside the template bullet.

➤ ***Note:** In the **Comment** window just under the list of templates, a brief description of the experiment is shown. This description can be entered into the **Comment** box of the **Cell Definition** page (the next page of the New Experiment Wizard).*

In the bottom window, the name of the experiment **MUST** be entered. With the database structure of PowerSuite, each record (containing all the data and formats for a given experiment) must be given a name prior to entering any data. This also means that once the experiment is in progress, the data will be entered in this record and does not need to be saved afterwards.

- **Note:** The name of this record will later appear in the « **Database Management** » tool.
- **Note:** « **Run on Finish** », if checked, will start the experiment automatically, as soon as you finish the New Experiment Wizard.

Click on « **Next** » to go to the next setup page, **Cell Definition**.

- **Note:** If you already know what the setup structure is, you can click « **Finish** » to jump immediately to the end of the New Experiment Wizard.

### 3-2: Cell Definition Window

This page lets you setup the conditions for an experiment.

« **Comment** » allows you to enter text comments for the experiment. Later, keywords from this text can be searched within the « **Database Management** » function (section 2).

« **Instrument** » allows you to select the potentiostat of your choice (since multiple potentiostats can be connected). If you have only one potentiostat, it is best to select AUTO.

« **Background Dataset** » allows you to select a record to subtract from the present data acquisition (PowerCV only).

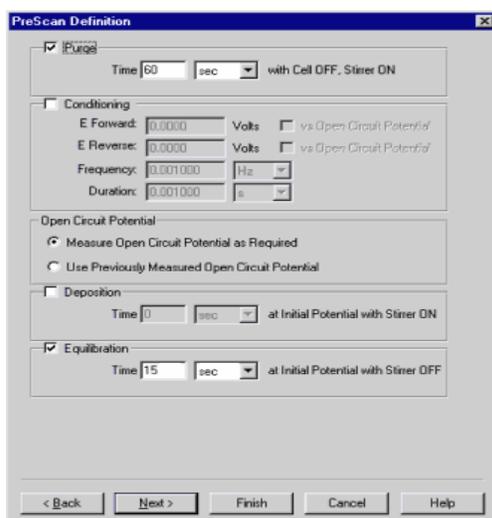
« **Working Electrode** » allows you to choose the type of electrode you are working with and specify the active area of your electrode.

« **Reference Electrode** » allows you to choose the type of reference electrode you are working with (or create your own type by clicking the button to the right of the drop down menu). Once this is specified, the software can later recalculate your data for different types of reference electrodes with the use of « **Graph Properties** ».

Click on « **Next** » to go to the **PreScan Definition** page of the setup.

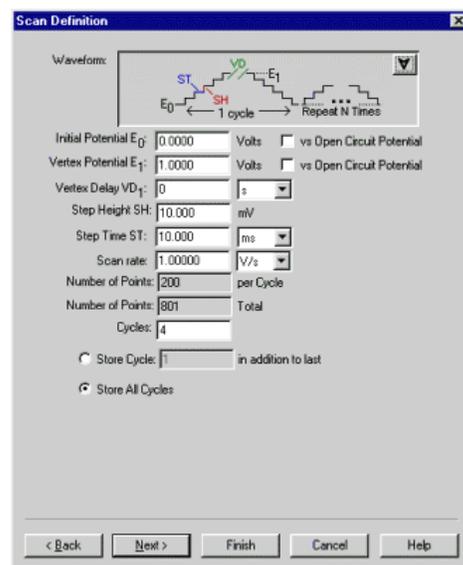
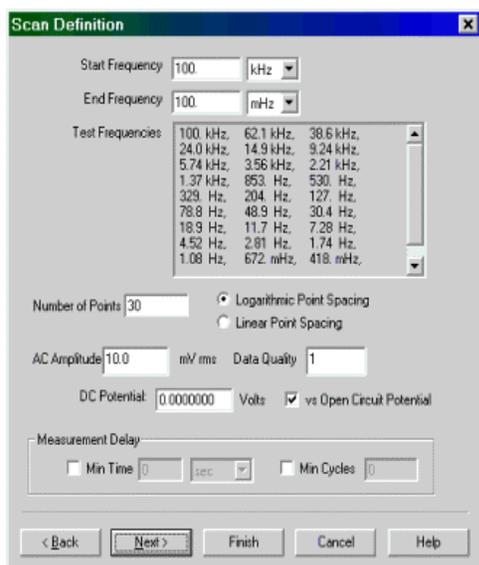
### 3-3: PreScan Definition Window

This window allows you to set some pre-experimental conditions, according to the type of electrode you are using. These settings will be executed in an automated sequence, prior to the actual start of the experiment. If you are using a SMDE controlled by the potentiostat, **Purge**, **Deposition** and **Equilibration** steps can be set. Unchecking the boxes allows you to skip these steps.



- **Note:** « **Conditioning** » allows you to pulse the electrode prior to the experiment with a SWV wavepulse and is often used for potentiostatic electrode cleaning purposes. When setting E Forward and E Reverse to the same potential, a constant potential will be applied.
- **Note:** Having « **Open Circuit Potential** », « **Measure...** » checked will measure the OCV prior to the experiment, while « **Use Previous...** » will automatically use the OCV from the previous experiment. This is often used in combination with the « **AutoExecute** » operation.

### 3-4: Scan Definition Window

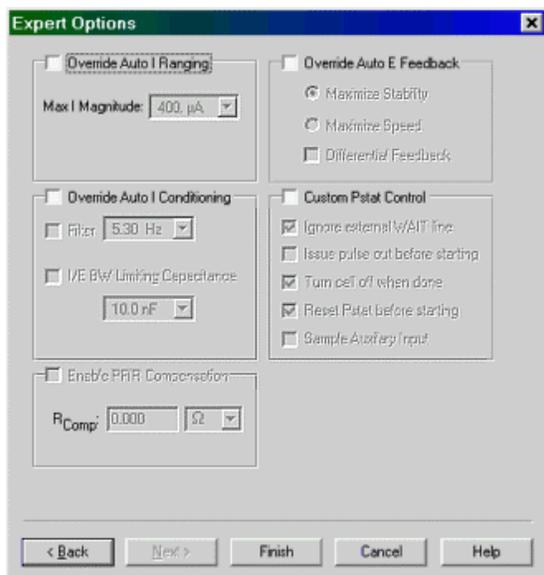


The

experimental parameter setup pages shown here depend upon the chosen technique. Default parameters will be proposed. For details and extended parameter information, consult the **Help** section of this software.

- **Note:** For PowerCV, a maximum of 1100 points per cycle can be obtained, with a maximum of 90 cycles. This is 100,000 points per experiment.
- **Note:** In the top right corner of the waveform window, the down arrow can be clicked in order to select a different waveform setup for the chosen technique.

### 3-5: Expert Options Window



« **Override Auto I Ranging** » allows you to fix the current sensitivity range of the potentiostat. By default, this box is not checked and the automatic ranging will be active. Check this box to allow a fixed current range to be chosen from the drop down menu.

- **Note:** « *Enable PFIR Compensation* » will only be active if a fixed current range is chosen.

« **Override Auto I Conditioning** » This function provides the use of different types and combinations of filters. By default (unchecked), no filters are active. When checked, you can choose the filters from the drop down menu.

- **Note:** Filter choices and combinations available are dependent upon the potentiostat model being used.

« **Override Auto E Feedback** » sets the bandwidth of the potentiostat. In normal operation, the **Auto E Feedback** should be in **Stability Mode**. This will reduce the chances of oscillation. It is best to leave the box unchecked so the default setting for the given potentiostat is automatically in use. More details can be found in the **Help** section.

« **Custom Pstat Control** » This allows you to set some special functions.

- « **Ignore external WAIT line** » controls an incoming trigger pulse from an external device. The potentiostat will wait to start the experiment until the external trigger is received.
- « **Issue pulse out before starting** » controls an outgoing trigger pulse. The potentiostat will send out a trigger in order to start the external device at the beginning of the electrochemical experiment.
- « **Turn cell off when done** » will turn the cell switch off automatically at the end of the experiment. In some cases, when consecutive experiments are programmed, you may want the cell to be turned on, even between running the succession of experiments.
- « **Reset Pstat before starting** » When checked, the potentiostat will be reset at the start of the experiment. This is the default setting. At this point, the external input switch (from the GPIB-controlled potentiostats) will be turned off. If you need this input to stay active

(to superimpose an external waveform during the experiment), this box needs to be unchecked.

- **« Sample Auxiliary Input »** At the back of the potentiostat is an external synchronized ADC input BNC connector. This allows data to be taken from an external device (such as a spectrophotometer, QCA, pH meter, etc....) and synchronized with the E, I, and t data from the experiment. Check this box to activate and allow the potentiostat to sample the external device's output.

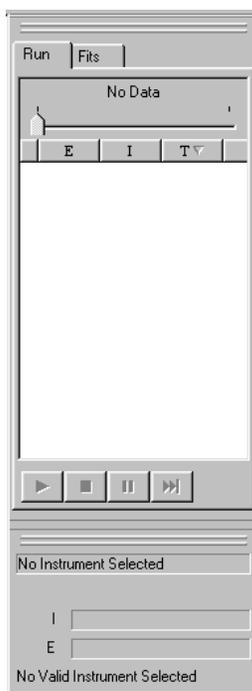
➤ **Note:** *In all modules except PowerCV, this function is automatically active and does not need to be turned on or off. In PowerCV it must be set manually.*

### 3-6: Finalizing the setup conditions

Once all the parameters have been set, click on **« Finish »** to begin the experiment execution phase. A default graph window will appear depending on the chosen technique or module (for example I vs. E for PowerCV). On the right hand side are two additional windows, the experiment bar and the instrument bar.

➤ **Note:** *If the instrument bar does not appear in the same position as in the picture below, you can drag and drop it into this position by clicking on the edge of the window.*

➤ **Note:** *Click on « View » in the top banner to set or change these windows. In « View », these bars can be unchecked which will maximize the graph size on the screen.*



At the very start, both windows will be inactive (as in the picture to the left).

- **Note:** *In the lower instrument bar, your potentiostat model with firmware version and serial number should appear (for example, PARSTAT 2263.02 SN103). If this does not occur, as in the picture to the left (No Instrument Selected), you should re-initialize your potentiostat through the « Tools », « Search for Instruments » function.*

At this moment, the software will load the experiment settings in the potentiostat. This appears as **Booting Pstat ...%**. **Caution: Do not force any other action until the booting process is complete.** Once completed, the instrument bar will become active, showing the cell on/off status, actual current range and I and E open circuit readings. In the experiment bar, the run button (arrow) will now be active.

- **Note:** At this point you can still make changes to your setup conditions. By clicking on « **Properties** » (the last button in the tool bar or through « **Experiment** », « **Properties** »), you will get an overview of the setup pages. They will all be active and can be re-adjusted if needed. Once the experiment has started, you can still view the experiment properties, but the settings will become inactive in order to preserve the conditions while the experiment is in progress.

Click on run (the arrow button) to start the experiment and data acquisition.

- **Note:** If you have previously set the **Purge, Condition or Equilibration** functions in your **PreScan Definition** setup page, you can skip these steps by clicking the skip button.

#### **4) Saving the experimental setup conditions as a template**

What was previously called « **SAVE SETUP** » under DOS software is now called « **Save As Template** ». It is not stored as a file (as was the case in DOS), but saved as a template within a database called « **Templates.mdb** ». This allows you to create templates for routine use later on.

- **Note:** The templates database is located under the Electrochemistry PowerSuite directory of your hard drive.
- **Note:** You can either store the setup template before or after running the experiment.

After the experiment has finished, click on « **Experiment** », « **Save As Template** » and give the template a suitable name (25 characters max). As soon as this is done, the saved template can be found and accessed through the **New Experiment Wizard**. The newly created template will be listed under the assigned technique, next to the already existing default templates.

#### **4-1: Deleting a previously stored setup template**

Open « **Database Management** » (section 2), select « **Templates.mdb** » as your source database, open the proper technique, click on the template you want to delete, and click the « **Delete** » button.

- **IMPORTANT:** In the list, you will also find the default setup templates. They are listed with (def) in front of their name. These default setup templates are not protected, so you should be careful not to delete one of the defaults. If you do, they will be gone completely from the templates database. Reinstallation of the software is needed to restore them.

#### **5) Modifying an experimental setup parameter when running consecutive experiments**

After running an experiment, you may want to modify a setup condition and repeat the experiment. There are two options based on whether you want to keep the previous data or delete it.

### **5-1: Storing the previous data, changing a parameter and repeating**

Since the actual data is already stored in the record (for example, you named it « test1 » in the **Choose a technique template** window), you need to create a new record to enter the new data (you could name it « test2 »). Go to « **Experiment** », « **Save As** » and enter the name « test2 ». Note that the name of the previous experiment, « test1 », has now been changed to « test2 » in the top left banner.

- **Note:** « **Save As** » in this sequence does not really mean that you are saving the previous data as « ... ». The data was already in the record so you don't need to save again. « **Save As** » now means start a new record. The previous record « test1 » has now been saved in your database.
- **Note:** At this point, you still see the « test1 » data on your screen. This is because it has not yet been deleted from the computer's memory. As a result, the parameters cannot be changed (Click on « **Properties** » and scroll through the different setup pages. You'll see that all parameters, still set to the « test1 » setup, are grayed out and cannot be modified).

In order to now make parameter changes, you first need to clear the screen of the data that is still residing in memory. Click on « **Edit** », « **DeletePoints** », and then select « **Entire Data Set** » and « **OK** ». Now the « test1 » data is cleared from the « test2 » record and you are ready to collect new data in « test2 ».

- **Note:** This last operation can be done by clicking on the first button of the experiment bar. 

Click on the « **Properties** » button, select the parameter you want to change, click on « **Finish** », and start the run again. The new data will now be entered in the « test2 » record.

### **5-2: Deleting the previous data, changing a parameter and repeating**

In this case, after « test1 » has finished, click on the « **Delete** » button of your experiment bar, click on « **Properties** », change the parameter and click on « **Finish** », **Run**. The « test1 » data is cleared and new data can be entered into the same record.

### **5-3: Deleting the previous data and repeating without changing a parameter**

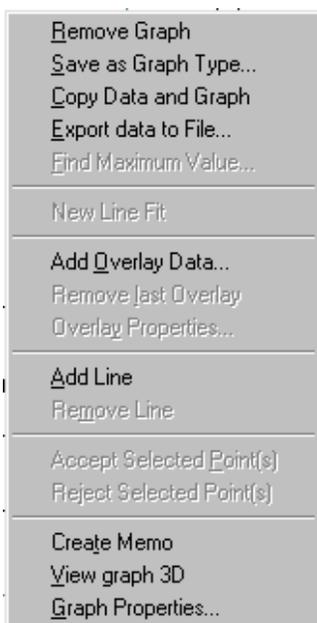
Just click on the « **Delete** » button and run.

- **Attention:** When modifying the parameters, these changes are not saved in the setup template. In order to save the new parameters as a template, re-save using the « **Save As Template** » function.
- **Note:** The « **Save As** » function can also be used to change the name of an already stored data record, BUT only when the data has been modified (for example, by deleting some of the points).
- **Attention:** Renaming a record 'as such' is not permitted in PowerSuite.

## 6) Graph Properties

PowerSuite uses a very powerful graphics platform. After creating a new method and having clicked on « **Finish** », PowerSuite will create a blank default graph, based on the chosen technique.

- I vs. E for Voltammetry (PowerCV)
- I vs. t for Chronoamperometry (PowerSTEP)
- E vs. t for Chronopotentiometry (PowerSTEP)
- Delta I vs. E for Differential Pulse Voltammetry and Square Wave Voltammetry (PowerPULSE)
- Nyquist, Bode Phase, Bode Z, Bode Phase and Z for Impedance (PowerSINE)
- E vs. Log I for Tafel (PowerCORR)

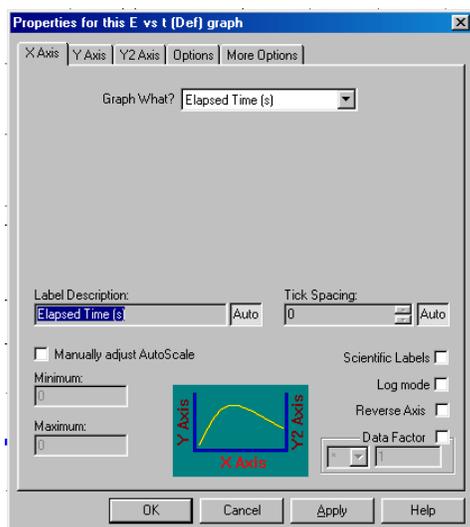


- **Note:** When you go through « Add new graph », a slightly different procedure will be followed (see the end of this section).

Each graph has its own associated properties that can be accessed and stored. You can access these properties by pointing the mouse on the graph of interest and clicking. This selects the graph (if there are more than one on the screen) making it active. Then, **RIGHT MOUSE CLICK** to view the graph settings options (figure shown at left).

The « **Graph Properties** » settings are accessed through a series of tabs. These properties will allow you to set the complete layout for the selected graph.

- **Note:** These graph settings will be stored automatically within the data record. Whenever you recall this data, it will be graphed in the format last viewed.

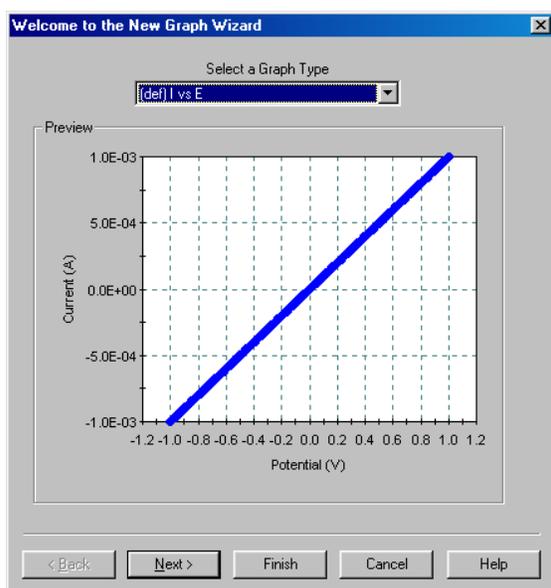


- **Note:** Once a particular graph configuration is chosen, you can save this format as a graph template for later use. This can be accessed through « **Save as Graph Type** » in the above window. The template is automatically stored in a separate database called « **Templates.mdb** » in the Electrochemistry PowerSuite directory.
- **Note:** In PowerCV, an extra window called « **Series** » will open first in order to setup the views for multi-cycle CV data.

## 6-1: Add new graph procedure

In your PowerSuite display, you can create up to 4 different graphs. All the graphs will be active during data acquisition. On the top banner under « **View** », click on « **Add new graph** ».

- **Note:** If you already have 4 graphs on your screen (by default in PowerSINE), the « **Add new graph** » function cannot be accessed since only 4 graphs maximum can be created. In this case you could choose to remove one of the graphs. Activate the graph that you want to remove by clicking on it with your pointer, right mouse click and select « **Remove Graph** ». Now you will be able to create a new graph.



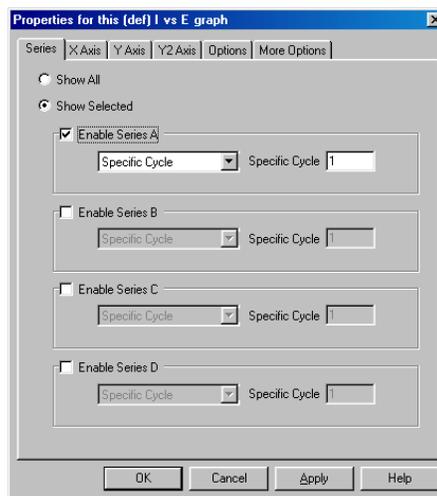
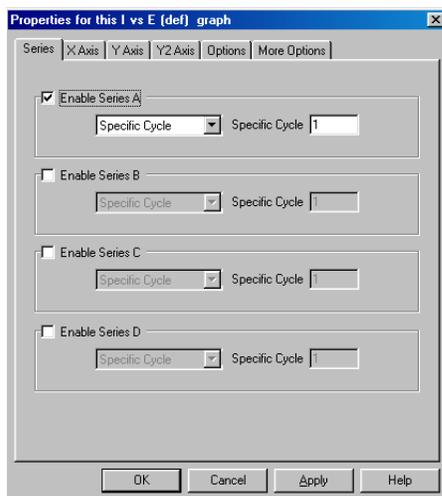
In the Welcome to the New Graph Wizard page, you can select the type of graph you want to add to your data set. By clicking on « **Select a Graph Type** » a range of graph type defaults will be shown.

- **Note:** If you have previously stored a graph template, it will show up here, in addition to the default list.

Once a graph type is selected, you can:

- Click on « **Next** », in order to change or re-define the graph settings.
- Click on « **Finish** », in order to skip the graph property settings wizard and create the default graph proposed by the welcome page.

## 6-2: Series (only for PowerCV data)

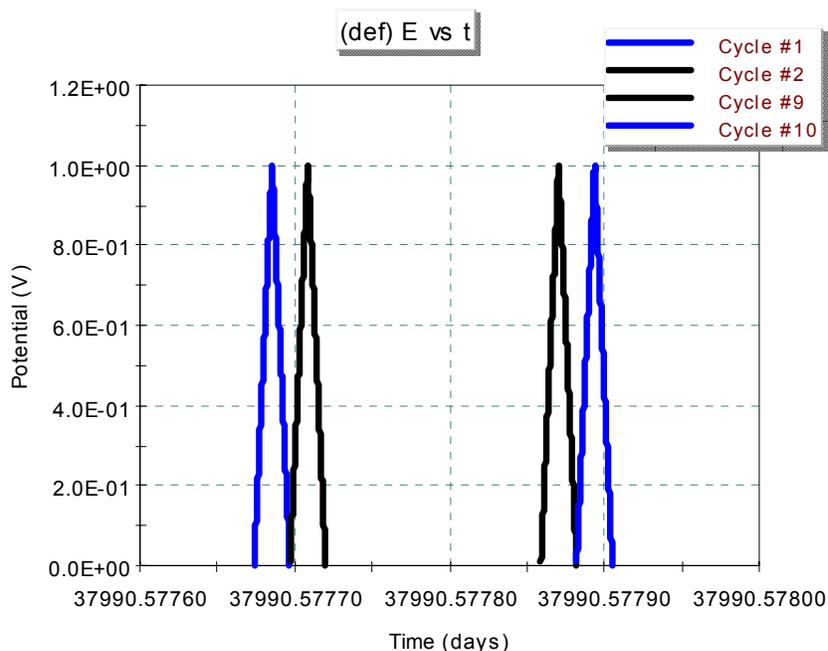


Left: PowerCV series window, before version 2.40

Right: PowerCV series window, starting from 2.40 on. *Note the « Show All » feature.* There are 4 sections. Each section allows you to set the number of the cycle you want to view in the graph. Up to 4 cycles can be viewed in one graph.

- **Note:** You can create up to 4 graphs of this type on your screen (a maximum of 16 cycles can be individually viewed).

By default, only 1 cycle, the first one, is selected. For example, if you have setup a CV to run 10 cycles, and you want to see the 1st, 2nd, 9th and 10th, you need to enable all 4 Series and set the « **Specific Cycle** » from series A to 1, B to 2, C to 9 and D to 10. Only these 4 cycles will be viewed. After finishing the experiment, you can view other cycles by changing the settings if you have selected « **Store All Cycles** » in the **Scan Definition** window.



If you want to see more than 4 cycles, you must either create a new CV graph with the extended settings, or use the « **Show All** » function.

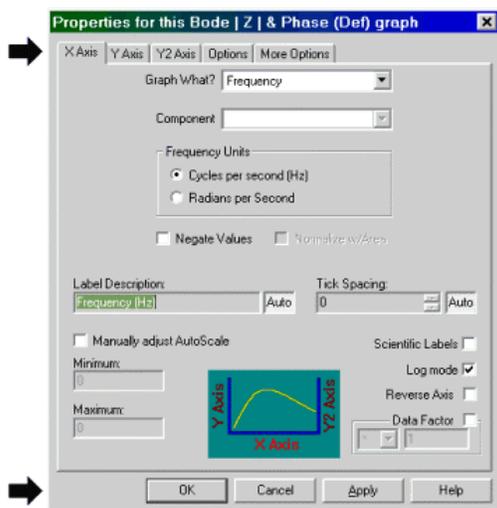
- **Note:** An easy way of mastering these views is to create an E vs. time (days) graph, where you can see the applied waveform displayed in time (figure above).

### 6-3: X Axis Tab

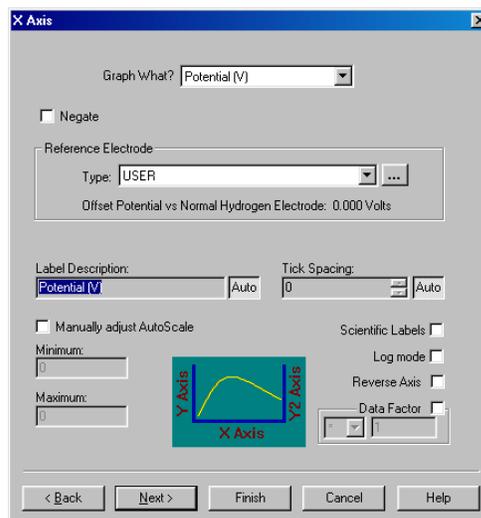
This is your definition of the X-axis. Click on « **Graph What?** » to select the parameter for your X-axis. Depending on the type of technique you have chosen, different options will be available.

- « **Label Description** » To change the label description, click on « **Auto** ».
- « **Data Factor** » allows you to setup a new axis definition. When you are sampling an external signal with the AUX A/D input from the potentiostat, you

can recalculate the incoming voltage signal with a factor representing the new parameter (for example, absorbance).



X-axis definition in PowerSINE



X-axis definition in PowerCV

- **Note:** To manually fix the scale of your axis, check « **Manually adjust AutoScale** » then enter the minimum and maximum values.
- **Note:** If potential is chosen, the reference electrode potential can be recalculated. This function will subtract the value of the chosen reference electrode. If you choose the same reference electrode as the one set in your **Cell Definition** page (section 3-2), there will be no shift in potential. Your label description will not be automatically adjusted for this change. You'll need to change the label manually.

#### 6-4: Y Axis Tab

Same as the X Axis definition.

- **Notes:** When the current is selected, 4 new items will appear:
  - « **Negate** » inverts of the sense of the plot.
  - « **Smooth** » smoothes the data with a sliding window averaging technique.
  - « **Normalize w/Area** » recalculates for the area ( $A/cm^2$ ), depending on the value entered for the working electrode surface area in the **Cell Definition** page (section 3-2).
  - « **Natural Log** » recalculates for Ln or Log of the current.
- **Notes:** Label descriptions will not be automatically adjusted for the changes.

#### 6-5: Y2 Axis Tab

Same as the Y Axis definition. By default, the Y2 axis is not shown. To show the second Y axis, check the box « **Show Axis** ».

## 6-6: Options and More Options Tabs

Allows you to design your graphs for presentation purposes by setting colors, text fonts and sizes, legend and title positions, grids, and backgrounds. In **Options**, the data can be represented as lines and/or dots. For multi-cycle CV data, different colors can be set for each of the selected cycles (section 6-2) in order to better resolve overlapping. More detailed descriptions can be found in the **Help** section of the software.

## 7) Graph Utilities

### 7-1: Graph scaling and positioning tools



- « **A** » signifies the **Autoscale** function. First click on the icon, move the cursor onto the graph and click again. Notice the 'A' sign in the top left corner of the graph, indicating the graph currently in view is fully autoranged.
- « **IN** » signifies the zoom in function. First click on the icon, move the cursor onto the graph, click and hold the mouse button, then drag the box around the section you want to zoom in on and release the mouse button.
- « **2X** » signifies the zoom out function and will zoom out by a factor of 2 for each click. First click on the icon, move the cursor onto the graph and click again.
- « **Move Data** » will allow you to reposition the data inside the graph by dragging. First click on the icon, move the cursor onto the graph (it will change to a hand cursor), click and hold while dragging the curve into another position.

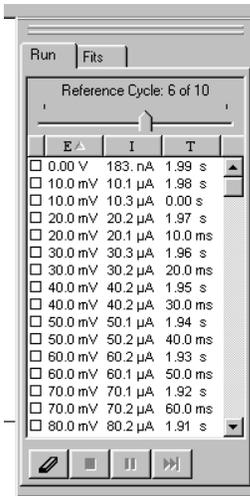
➤ ***Note:** All these functions can be repeated consecutively.*

### 7-2: Selecting data points

In order to select (or activate) a range of data points, move your cursor to the position on the graph where you want to select the range. Left mouse click, hold the mouse button and drag the rectangle over the data points. Release the mouse button. The selected data will show up highlighted in red. Note that this action will take place in all graphs at the same time. Also note that the selected range of data points will be highlighted in the experiment bar (to the right of the graph).

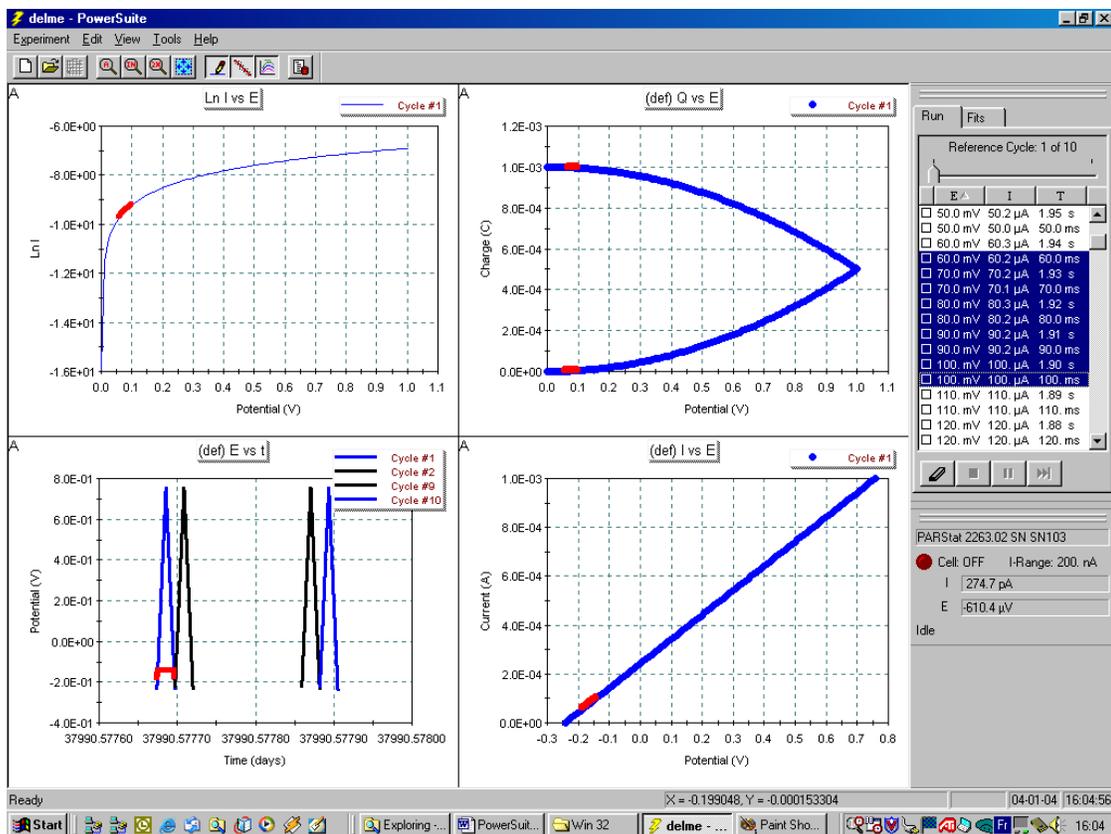
➤ ***Note:** In « **View** », **Experiment Bar** needs to be checked in order to view this window.*

➤ ***Note:** Data points can also be selected within the experiment bar's data table. Just click on the data point or use the control or shift key to select a range of points. These data points will now be highlighted in all graphs. This allows you to see where the selected data point is positioned.*

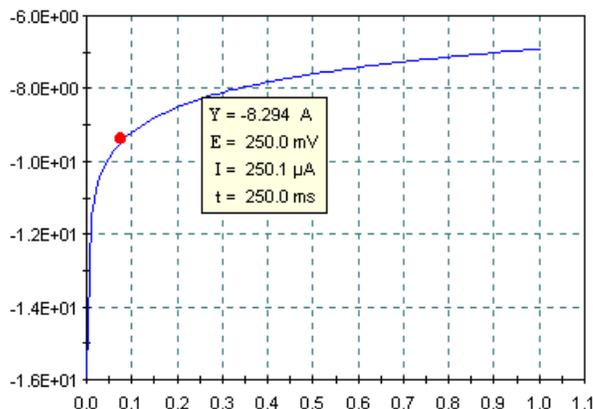


**Note:** In the experiment bar (shown to the left), the **Run** tab shows the list of all the data points. You can sort these data points by clicking on the parameter tab (**E**, **I** or **T** in the left example). If the data are generated from a multi-cycle CV, each cycle can be viewed separately.

The figure below gives you an overview of all these features and how they look on your screen.



The « **Hover Box** » shows each individual data point's content. Just position your mouse pointer exactly on the location of the data point you want to see and automatically a hover window will open, showing all data point information. The information will be dependent upon the type of graph you have selected.

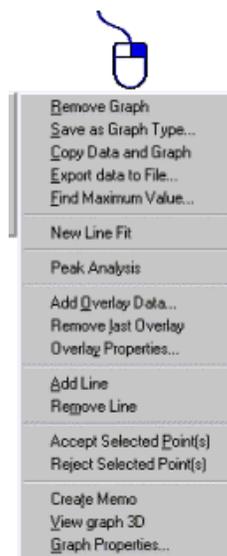


➤ **Note:** For a CV experiment, the hover box will also show the charge information, IF the data point has been selected.

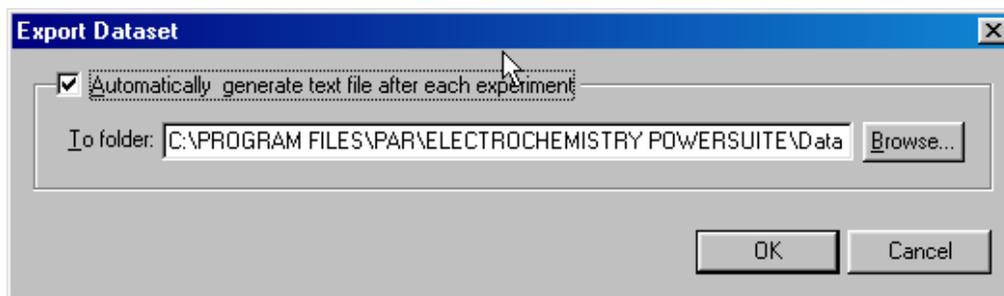
### 7-3: Right Hand Mouse click graph features

When you position the mouse pointer onto the graph of interest and right hand click on the graph, a whole range of options will become available. These options refer only to the graph you selected.

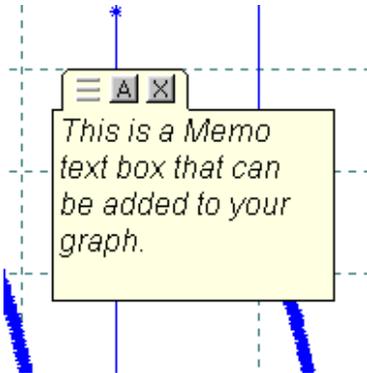
- « **Remove Graph** » allows you to remove the selected graph from the screen.
- « **Save as Graph Type** » allows you to save all the graph settings as a template (see section 6).
- « **Copy Data and Graph** » exports your data and graphs for quick reporting. (see section 9 and the last section of the addendum for an example of this).
- « **Export data to File** » exports the data from X and Y axes of the graph into a plain ASCII text file. (see also section 9)



➤ **Note:** This function can be automated, so that a text file will be generated at the end of each experiment. To access this feature, click on « **Tools** », « **Export data Set** » (only available from version 2.40 on).



- « **Find Maximum Value** » searches the maximum value of the Y component in your graph. Select the range of data points for which you want to find the maximum. Then right mouse click on the graph and select « **Find Maximum Value** ». The data point corresponding to this value will be highlighted in all graphs, as well as in the data table. You can either read this value in the data table or with the Hover Box. This point will be the maximum value on the Y-axis, independent of its sign.
- « **New Line Fit** » see section 8
- « **Peak Analysis** » see section 8
- « **Overlay Data** » see section 7.4
- « **Add Line** » « **Remove Line** » serves to add or remove a straight line on the graph. If the status bar is visible (if not, go to « **View** » and check the status bar box), the results from slope and intercept calculations of this line will be visible on the bottom left side of the status bar. The slope and position of the line can be moved using the end point dots on the line. Just drag and drop the endpoints where you want.
  - ***Note:** More than one line can be created in the same graph.*
- « **Accept & Reject Selected Points** » see section 7.5
- « **Create Memo** » allows you to create a memo box inside the graph, where you can add additional information. The box will be exported, along with the graph as a picture file, so it is retained in your reports. You can also cut and paste the experiment properties into this box. The fist icon serves to drag and drop the box anywhere inside the graph. The « **A** » is the text font editor. The « **X** » deletes the memo from the graph

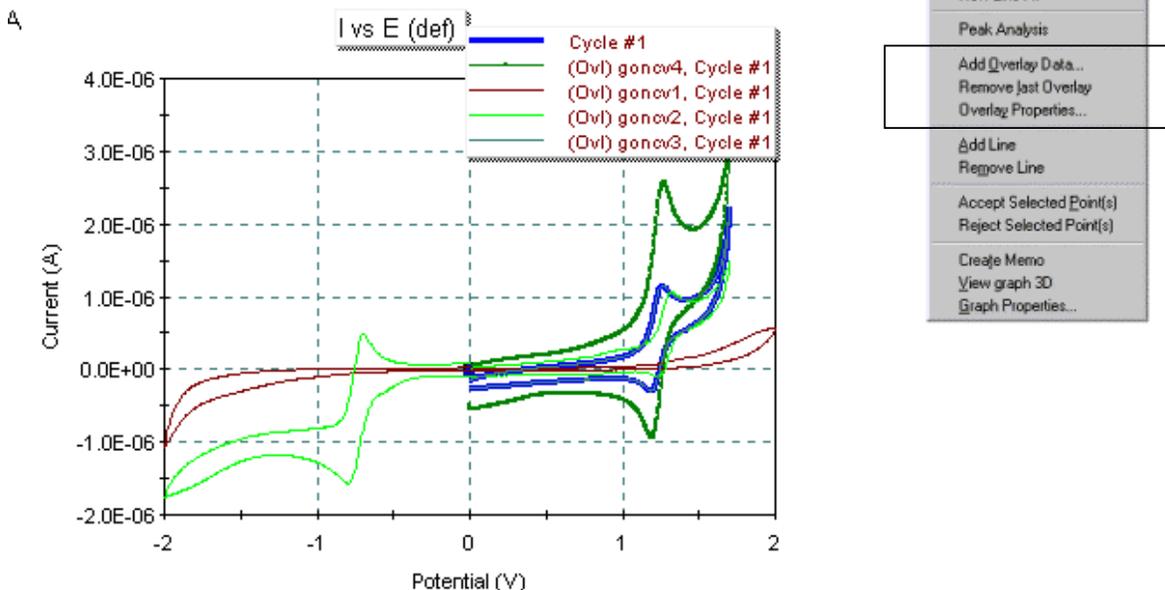


- ***Note:** You can create as many memos as needed. Copy your setup into the box by clicking « **Experiment Properties** », « **Copy** ». Then create a memo and click on « **Paste** ». The window of the memo box is not printed, only the text.*

- « **View graph 3D** » is only available for the Nyquist plots. Overlay several curves, then click on the 3D function. You can twist the 3D picture by moving the edges.

## 7-4: Overlay functions

Before you start working with overlays, make sure « **Overlay View** » is checked in the « **View** » tab. If it is not, overlays will not be visible. In each graph, you can create as many overlays as you like. However, they must be of the same technique.



- « **Overlay Properties** » (starting with version 2.3) This function allows you to modify the colors, lines and symbols of each overlay separately.
- « **Activate Overlay** » (starting with version 2.3) Only one overlay in a graph can be active, allowing you to select or reject points and calculate properties. To activate an overlay, click « **View** », « **Activate Overlay** ». At this point, you can choose which of the curves will be your ‘active’ data.
- « **Remove Last Overlay** » As soon as you have created one overlay, the « **Remove Last Overlay** » function will become active. It will remove the last overlay created.

➤ **Note:** When working with overlays, all graph windows that you have created on the screen will show the overlays.

## 7-5: Removing or Deleting Points from your graph

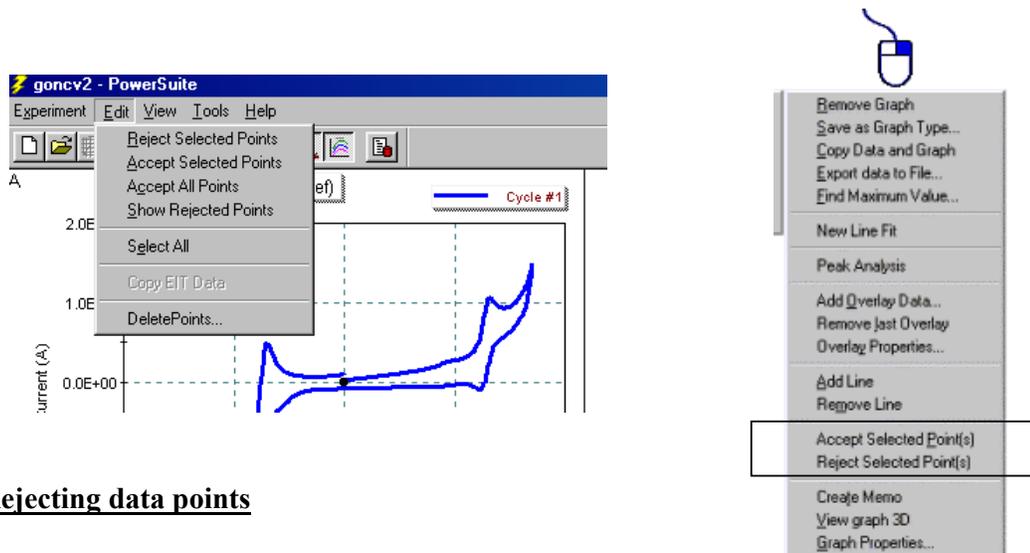
Data points may be removed from a graph by either temporarily rejecting the points, or permanently deleting the points. When rejecting, the data points will still exist but they will be removed from view. They can be added back to the graph at any time. When deleting, the data will be permanently deleted from your original record.

➤ **Note:** When you perform calculations on your data (smoothing, tracing a line etc...), the calculations will be performed on all data points in the record, even if they have been rejected from view. If you want your calculations NOT to include these rejected data points, you will need to use the « **Delete** » option.

Both of these functions can be performed on a single data point, on a range of selected data points, or on the complete data set. To do so, it is necessary to select a data point, a range of points or all the data.

All these functions are available under « **Edit** » on the top tool bar.

- **Note:** *The rejection function is also available through a right mouse button click on the graph. This allows you to quickly reject or accept the selected data. In this case, select the data on your graph, right mouse click and choose « **Reject Selected Points** ».*



### 7-5a: Rejecting data points

After data acquisition, either:

- Select one point
- Select a range of points
- Click on « **Edit** », « **Select All** »

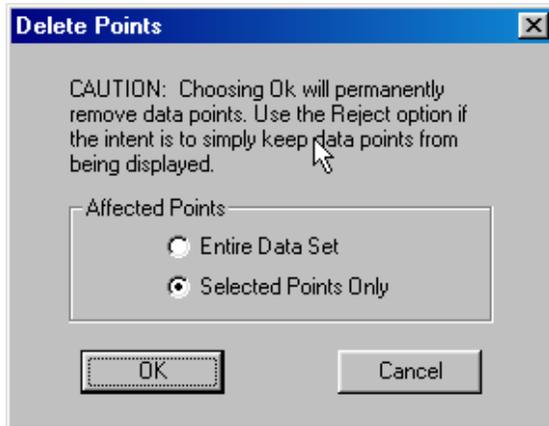
Click on « **Edit** », « **Reject Selected Points** ». At this time you can choose to view the points that you have rejected. To do so, click on « **Edit** » and check the « **Show Rejected Points** » function. Now your rejected points will be visible in different dot format.

### 7-5b: Getting rejected data points back in the graph

- Select a range of points a little wider than the range you rejected and click on « **Edit** », « **Accept Selected Points** »
- OR
- Click on « **Edit** », « **Select All** »
- then
- Click on « **Edit** », « **Accept All Points** », to get all the original data back into the graph.

### 7-5c: Deleting data points

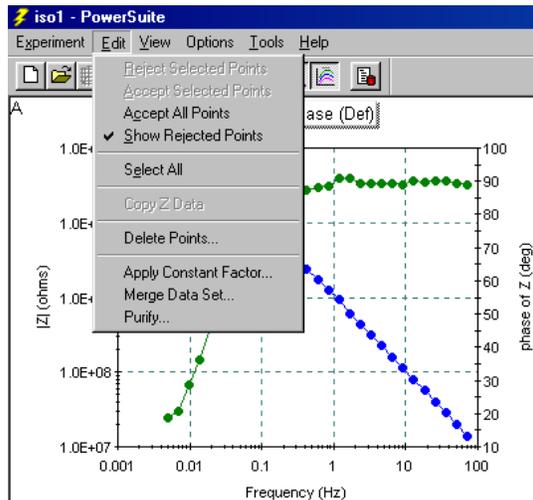
Select the data point(s) you want to delete, then go to « **Edit** », « **DeletePoints** ». There are two choices:



Check either « **Entire Data Set** » to delete all the data points, or « **Selected Points Only** » to delete the selected range or point. Click on « **OK** ».

**CAUTION: Using the deleting function PERMANENTLY removes the data record.**

- **Note:** In PowerSINE, click on « **Edit** », « **Purify** ». This operation will restore all rejected data points. This operation also restores any mathematical (« **Apply Constant Factor** ») and merging operations (« **Merge data set** ») previously performed.



## 8) Data Analysis

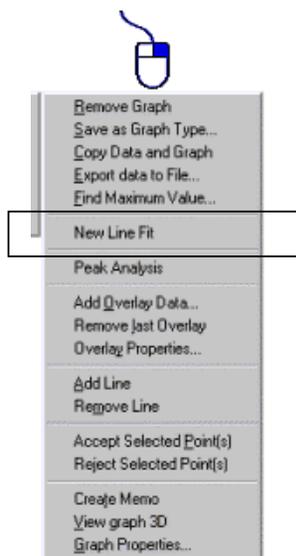
For data analysis, PowerSuite offers a whole set of tools to perform

- Line Data Fitting
- Peak Analysis
- Data Calculations

The procedures will depend on the type of technique (or PowerSuite module) you have created your experiment with. The analysis procedures include calculations on the data points themselves.

## 8-1: Line Fitting

The line fitting procedure serves to calculate the linear regression of a selected range of data points. It is a straight forward Linear Least Squares Fitting procedure, no matter what shape the data.



On the graph where you want to perform the line fit, select the range of data points to perform the fit on, then right hand mouse click on the graph and select « **New Line Fit** ».

A straight line will automatically be drawn through the selected range of points, and the calculation results will be shown in the **Fits** tab of the experiment bar on the right side of your screen (make sure this bar is visible by checking « **Experiment Bar** » under « **View** »).

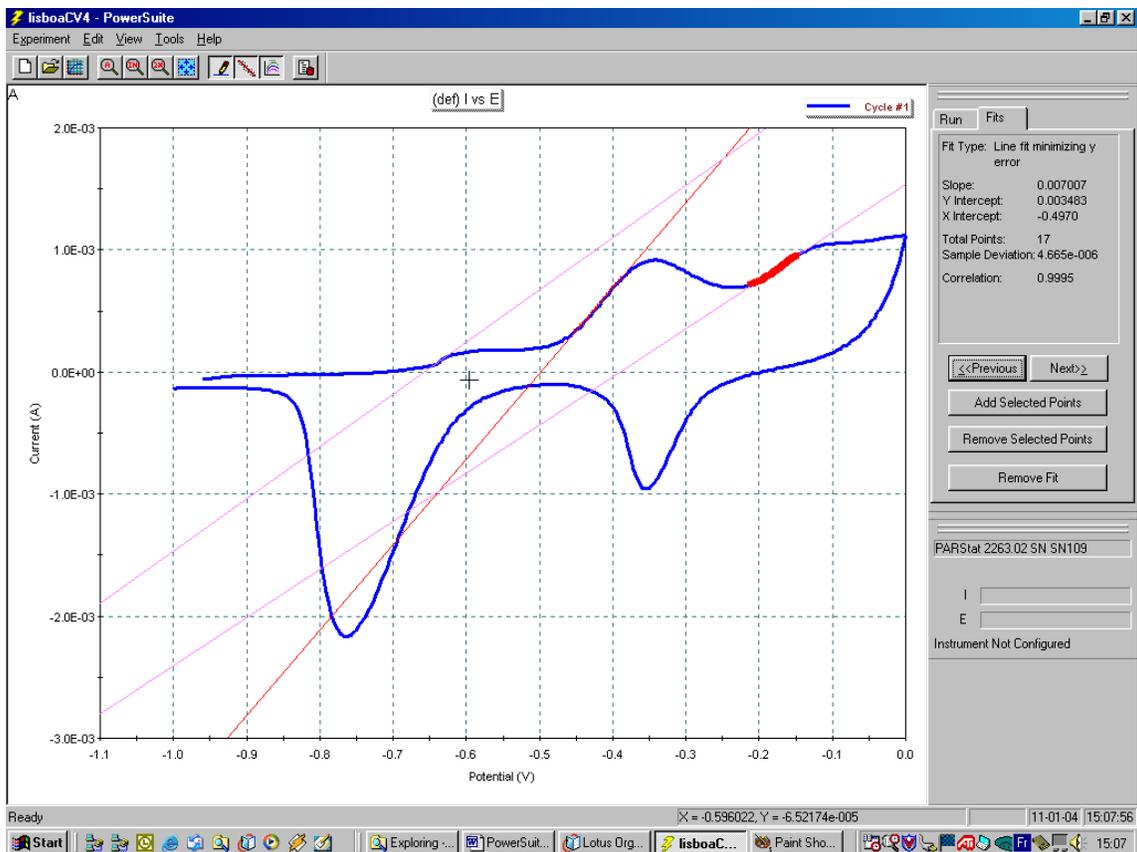
You can make several different fits on the same graph by repeating the above procedure. If you have drawn different fits, you can scroll through the fits using the « **Previous** » and « **Next** » buttons. The results shown in the **Fits** tab are the ones from the ‘active’ fit data. The ‘active’ fit line shows up in red, while the others are pink.

- **Note:** You can copy the fit results to your clipboard by right mouse clicking in the **Fits** tab window (see section 9.4)

Removing the fits and their results can be done by clicking on « **Remove Fit** » in the **Fits** tab window.

« **Add and Remove Selected Points** » serves to extend the selected range of data points that are included in the fitting process.

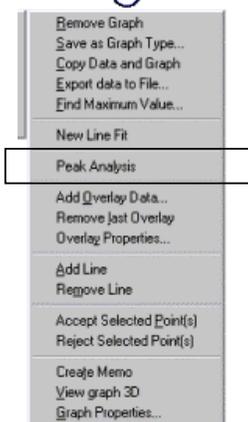
- **Note:** If the correlation of the fit with the data is not very good, the fit line will show a hatched surface between the data and the fitted lines.
- **Note:** « **Line Fit** » is different from « **Add Line** », « **Remove Line** » (see section 7.3). The Line Fit is not a line overlay. It is calculated on the data points themselves. The results do not show in the status bar.



## 8.2: Data Analysis

Data analysis is performed using « **Peak Analysis** » by right mouse clicking on the graph. The functions performed through this operation depend upon the type of experiment performed. First, you need to select the data points (all or a selected range), then right mouse click on the graph and the data analysis functions will become available.

In **PowerCV**, **PowerSTEP** and **PowerPULSE**, data analysis functions are listed under « **Peak Analysis** » and can perform following tasks:



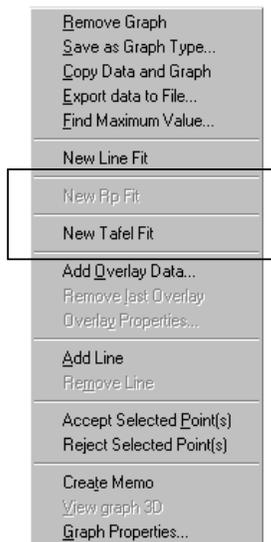
- Peak maximum current and potential
- Peak Full Width at Half Maximum (FWHM)
- Peak Area

At the same time, information will be given on:

- Voltage range of the selected peak data
- Slope of the baseline
- Offset current of the baseline (Y intercept)

➤ **Note:** Peak analysis is not available for the recurrent techniques in the **PowerPULSE** module.

In PowerCORR, data analysis functions are listed under « **New Rp Fit** » or « **New Tafel Fit** » and will perform following tasks:



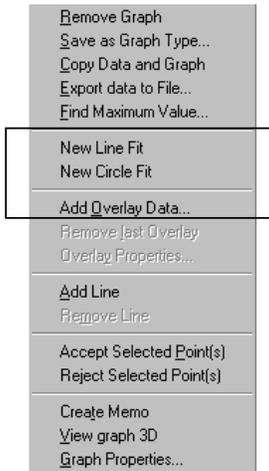
- Tafel Fits are available if the graph is shown as a Tafel Curve ( E vs. Log I ).
- Linear Polarization Fits are available if the graph is shown as a linear graph ( E vs. I ).

➤ **Note:** Potential must always be on the Y-axis and current on the X-axis AND be in the correct linear (for Rp) or log (for Tafel) mode in order to perform these functions. If they are not, « **New Rp Fit** » or « **New Tafel Fit** » will not be active or accessible. You will need to change the properties of the graph to put them into the correct display mode.

At the same time, calculated information will be given on:

- Ecorr (or Eoc)
- Icorr
- Anodic and Cathodic Tafel Constants
- Corrosion Rate
- **Note:** Equivalent weight and density of the material need to be entered in the **Cell Definition** window of the experimental setup in order for this calculation to work.
- Chi-Squared fitting quality parameter
- Fitting potential range.
- **Note:** On the graph, the Beta Lines will be visible and manually adjustable.
- **Note:** A right mouse click on the fit results will allow you to toggle between « **mpy** » and « **mmpy** ».

In PowerSINE, data analysis functions are listed under « **New Line Fit** » and « **New Circle Fit** ». « **New Circle Fit** » is only available for the Nyquist plots.

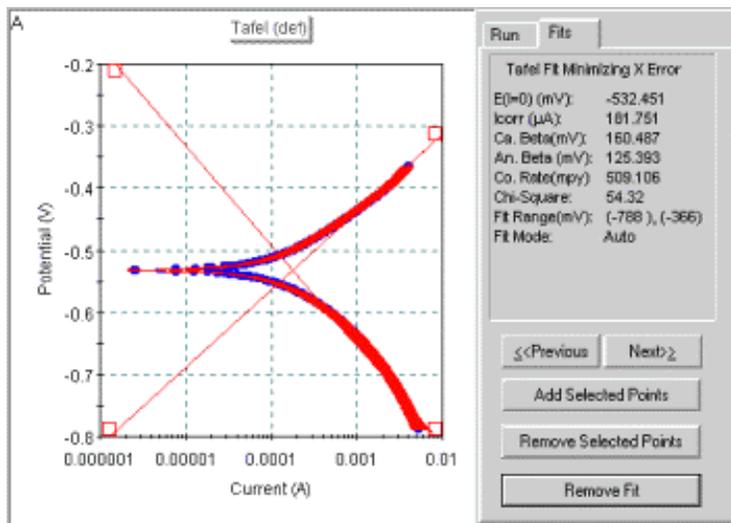
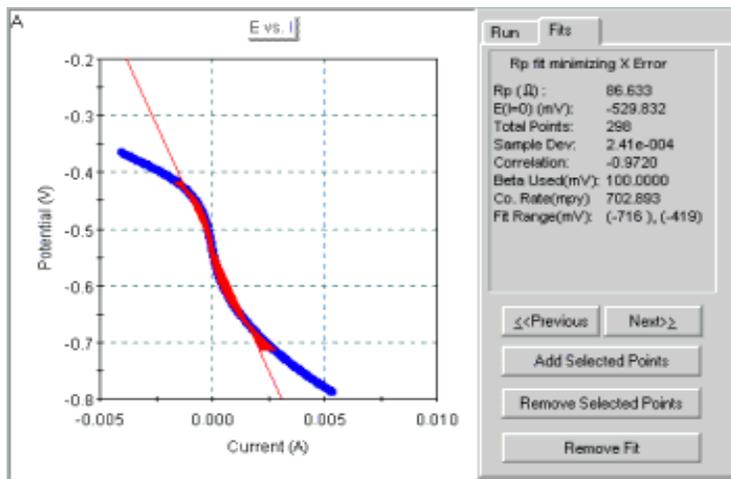


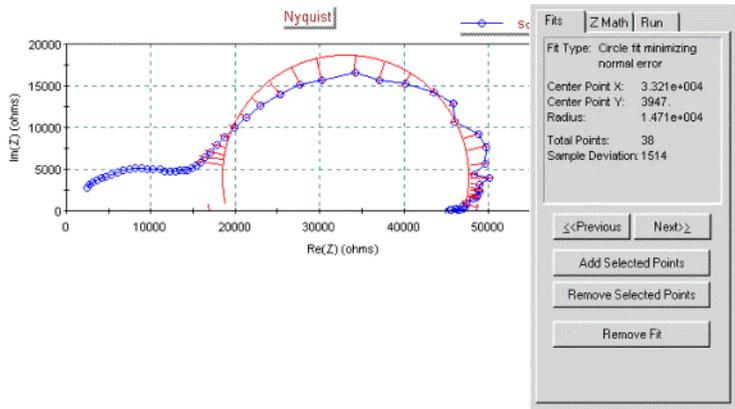
In PowerSINE, an extra tab will appear in the experiment bar called « **Z Math** ». This provides an extra tool to manually add or subtract R, C, L, RC and Z components from the equivalent circuit.

The Fit tab will provide statistical information on either the Circle or Line Fit calculation that you have performed.



EXAMPLE GRAPHS:





- **Note:** A separate software package called **ZSimpWin** can be purchased to fully automate equivalent circuit modeling. More information is available on the PAR website

**A fully detailed description on how and why to perform these data analysis techniques is available in the HELP section of PowerSuite.**

## **9) Data Export / Import**

Exporting data can be done in several different ways:

- Exporting data and graphs with the use of copy & paste
- Exporting to text format, ASCII files
- Exporting to a particular format ready for import into external calculation software.

### **9-1: Copy & Paste Procedure**

The simplest way to export data is to copy and paste your data and graph into an external ODBC compliant software package (like Excel or Word).

- Right Hand click on the graph you want to export, click on « **Copy Data and Graph** ».
- Start the Excel software.
- Click « **Paste** » to paste your ASCII data  
AND/OR
- Click on « **Paste Special** » and select « **Figure** » to paste the graph.

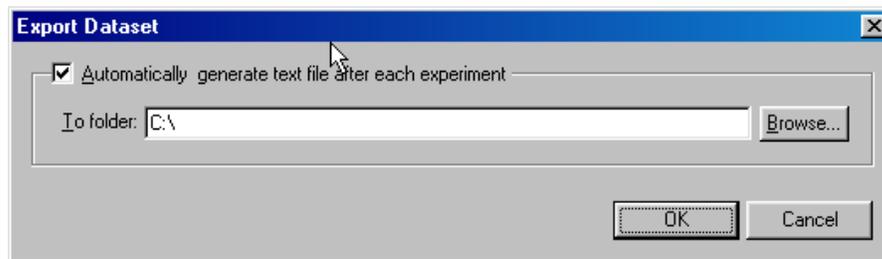
- **Note:** An example of this is given at the end of the addendum.
- **Note:** This function does not work on a selected data range. ALL the data will be exported (unless you have deleted them previously).

### **9-2: Data Exporting in Text Format**

#### **9-2a: Automatically generating a text file**

It is possible to request the software to create a text file of your data before the actual experiment starts. This way, a text file will be created automatically at the end of the

experiment. Simply choose « **Tools** », « **Export DataSet** » before you start the experiment and select the location for the file. If you want this operation to be executed for all your experiments, check the « **Automatically generate text file after each experiment** » box.



### **9-2b: Creating a text file from your graph data**

To create a simple ASCII text file from your graph data, right hand click on the graph you want to export, click on « **Export data to File** » and choose the location where you want to store the file.

- **Note:** Only the X and Y data (not Y2) from the selected graph will be exported.
- **Note:** Exporting a selected range of data is not possible.
- **Note:** This function can be fully automated (see section 7.3 « **Export to File** »)

### **9-2c: Exporting E, I and t data into a spreadsheet**

In your graph, either select a range of data points or choose « **Edit** », « **Select All** ». Then click on « **Edit** », « **Copy EIT Data** ». Either the selected range or all the data will be exported to the clipboard, ready to paste into an external ODBC compliant software.

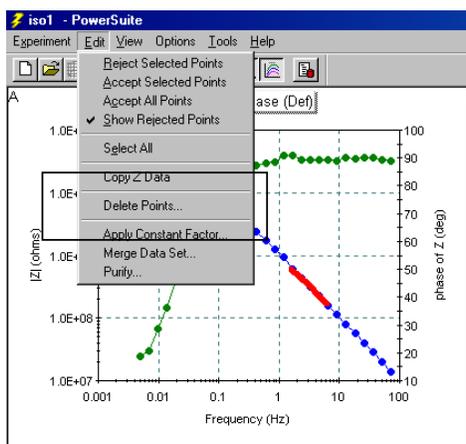
- **Note:** This function is not available in PowerSINE.

### **9-3: Exporting directly into ZSimpWin or CondeCon software**

#### **9-3a: Exporting into ZSimpWin**

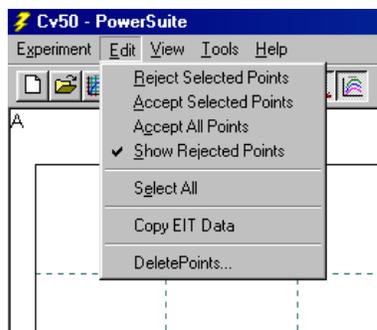
ZSimpWin is a software package (external from PowerSuite) to model equivalent circuits of your PowerSINE data. PowerSINE will allow you to directly export your data into ZSimpWin.

Select the full range of data points in your graph with the mouse selector (rectangular zoom). Click on « **Edit** », « **Copy Z Data** ». At this point, your data will be copied to the Windows clipboard and is ready to import into ZSimpWin. Only Frequency, Z Real, and Z Imaginary data are copied. Start the ZSimpWin software and paste the data.



➤ **CAUTION:** Do not use « **Select All** » or choose only a range of data points to export. These functions will give errors, « **invalid data on clipboard** », at the moment of import into ZSimpWin (version 3.10). ALL the data must be chosen.

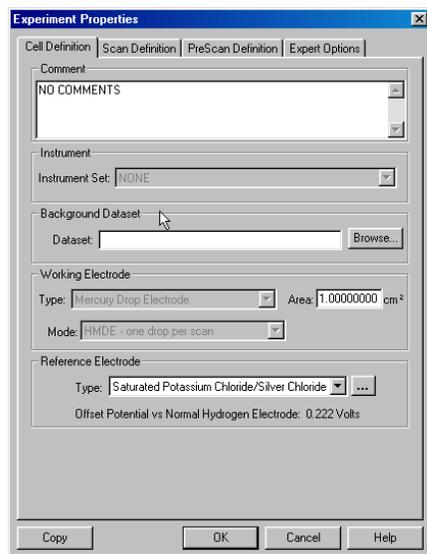
### 9-3b: Exporting into CondeCV and CondeSTEP software



CondeCV and CondeSTEP are powerful calculation programs to Convolute and Deconvolute CV and CA data. These programs provide electrokinetic modeling calculations.

Select the full range of data from your PowerCV or PowerSTEP experiment. Click on « **Edit** » then « **Copy EIT Data** » in order to prepare the data for import into either CondeCV or CondeSTEP.

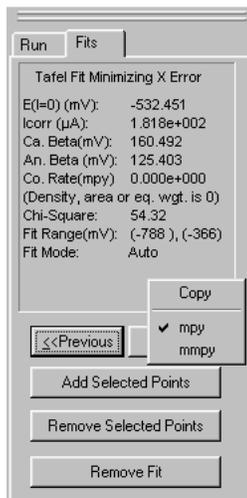
### 9-4: Exporting experiment properties



Either click on « **Experiment** », « **Properties** », or click on the **Properties** button on the tool bar (make sure the Tool bar is visible through the « **View** » button) to open the properties window.

On the bottom left side of the window is a « **Copy** » button. Click on it to export your experimental setup (that is the one that belongs to the data on your graph) in the Windows clipboard. It can now be pasted into any other software for presentation purposes.

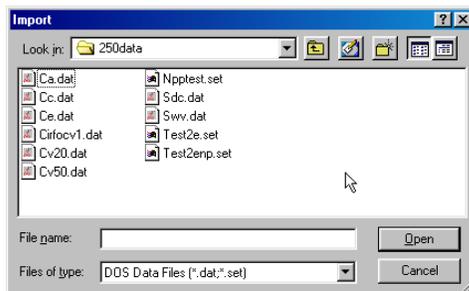
## 9-5: Exporting calculated results



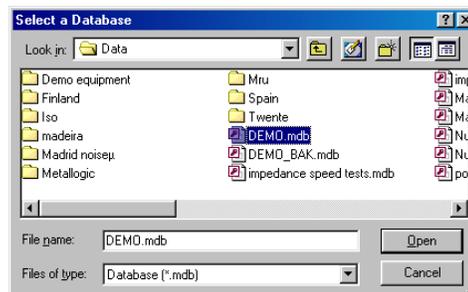
Select the **Fits** tab in the instrument bar to show the results. Place the mouse pointer on the instrument bar window. Right Hand click to show the « **Copy** » window and click « **Copy** » to export your fitting results into the Windows clipboard. It can now be pasted into any other software for presentation purposes.

## 9-6: Importing data

One of the features of PowerSuite is the ability to import data from the old DOS packages (M250, M270, M352, M398 or SoftCorrIII).



To do so, click on « **Tools** » then « **Import DAT Files** ». This window allows you to select the DOS files you want to import into PowerSuite. You can select as many files at one time as you like. Then click « **Open** ».



Next, select the database into which you want to import the selected DOS files.

- **Note:** It is wise to create a new database to separately store the old data before beginning the import procedure (see « **Database Management** », section 2).
- **Note:** You can only select a proper database from this list. Creating one by entering a new name here will not work. This needs to be done in « **Database Management** » under « **Tools** ».

Click on « **Open** » and the software will start recalculating the data to import into the selected database. If successful, the following message will appear « **x files successfully imported** ». If the import is unsuccessful, it is probable that your data was not stored in the correct DOS format.

The following message may appear:



When successful, the data will be inside the chosen database but no graphic display has been attached yet, so nothing will appear on your screen.

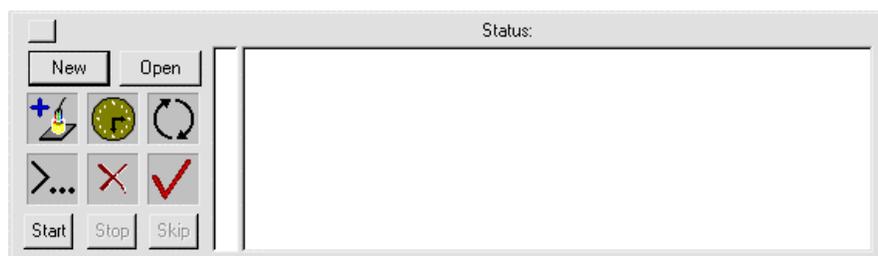
To view the data, click on « **Experiment** », « **Open Data Set** » or click the « **Open** » button on the task bar. Select the database you have chosen to store the imported data, open the technique (which should be the same as your original DOS file(s)), select the record you want to view and click « **Select** ». At this point, no graph will be shown since the graphical information was not contained in the exported data. PowerSINE will need to create these. You will need to setup a new graph to show the data. Click on « **View** », « **Add New Graph** », then edit the graph properties (as in section 6) or click on « **Finish** » if the default properties are ok. Now the graph will be on your screen for further enhancement and the graph properties will be stored along with the imported data.

- **Note:** You can only import data from a similar technique as the PowerSuite module installed on your computer will provide (PowerCV for M250 or M270 ; PowerSINE for M398 ; PowerSTEP for M250 or M270 ; PowerCORR for SoftCorrIII and M352 and PowerPULSE for M250 or M270). For example, importing a SWV (M250) experiment into PowerSuite will not work if you do not have PowerPULSE installed.

## 10) AutoExecute

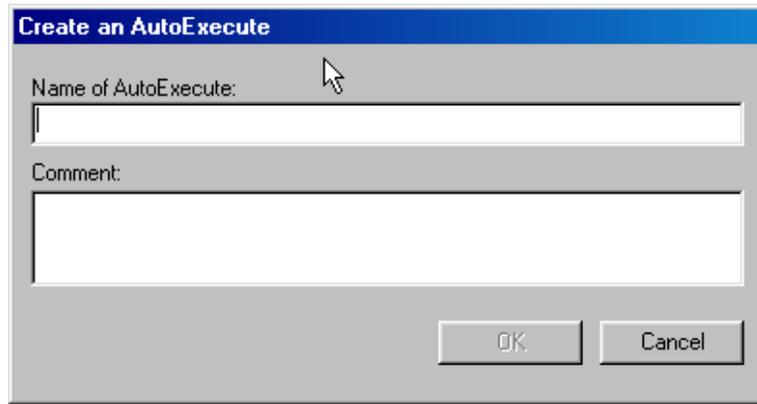
PowerSuite contains a function called **AutoExecute** that allows you to perform different experiments in sequence without user intervention. The chained experiments can originate from any module or technique installed within the PowerSuite software. AutoExecute uses ready-prepared experimental templates that will be executed sequentially, without user intervention. Such a complete programmed sequence can be given a record name and stored within an active database. This way, many different AutoExecute records can be created, stored and recalled. Within the AutoExecute program, timing and sequencing loops can be inserted.

To access the AutoExecute setup, you first need to click on « **View** », « **AutoExec Bar** ». The AutoExecute window will look as follows:



## 10-1: Command Buttons

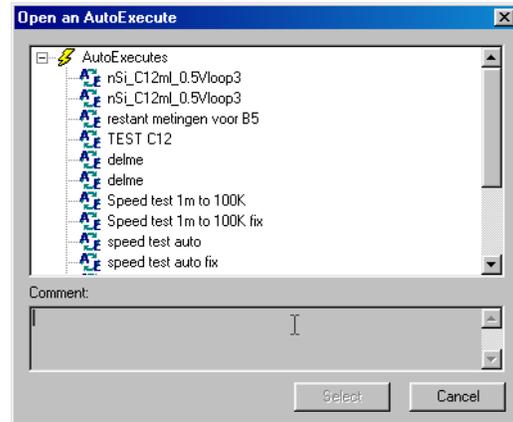
« **New** » will create a new autoexecute record. Click on « **New** ». Fill in the name you want to give the autoexecute that you are about to create (You can also enter some text into the comment box).



- **Note:** As soon as you click on « **OK** », an autoexecute record (with the given name) will be created. Then the sequence you want to create can be entered into the record. It will not be needed to store anything afterward.

« **Open** » opens a window with previously stored autoexecute procedures. Highlight the autoexecute of your choice and click on « **Select** ». This will load the selected autoexecute into the main AutoExecute window

- **Note:** The autoexecutes are embedded in the « *templates.mdb* » database, and cannot be exported or viewed as separate files or directories.



« **Start** » starts the autoexecute sequence.

« **Stop** » stops the sequence in execution

« **Skip** » stops the line in execution (which is given by the « > » sign in front of the line), and steps to the next line to continue execution of the sequence.

« ... » allows you to change the name of the autoexecute.

## 10-2: Command Icons

The icons are used to enter a sequence of experiments into AutoExecute. They are entered line by line into the right side status box of the AutoExecute window. This is done by a drag and drop operation. To use the icon function, left click on the icon and hold the mouse button (a '+' will appear beside the pointer). Move the cursor into the status box and release the mouse button.

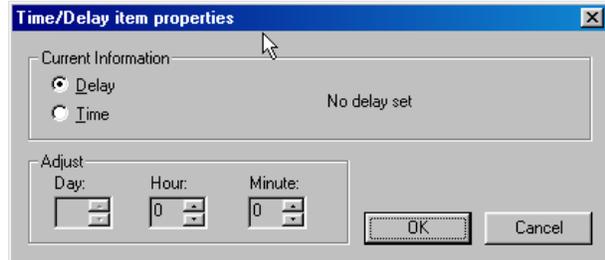


Experiment Select icon is used to select the technique and experiment template. The window also lets you setup the database into which the results of the selected experiment will be stored.

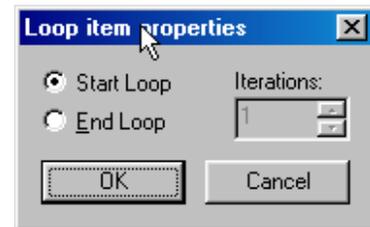
- **Note:** *Auto-Increment will add a number to the record name corresponding to the loop number.*



Timing icon is used to enter timing and delay pauses into the sequence. It will allow you to either insert a delay time between two lines or insert a time at which to step to the next line.



Loop icon is used to create a loop between different lines, as well as the number of times the loop needs to be executed (Iterations). Both the start and stop lines need to be dragged and dropped separately (and in sequence) into the status box.



Text Line icon serves to enter a line of text (80 characters max) in the sequence.

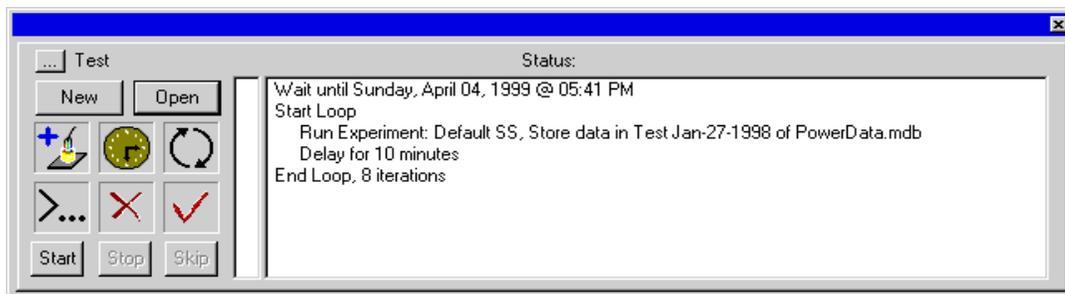


Delete Line icon serves to delete a line from the sequence.



Verification icon will diagnose if there are any timing incoherencies in the sequence.

**Example:** This is an example of an autoexecute called « **Test** ». When clicking the « **Start** » button, the software will wait until 5:41 PM on April 04, 1999. Then it will start to run the experiment template called « **Default SS** ». The data will be stored in the « **PowerData.mdb** » database under the record name « **Test Jan-27-1998** ». Upon completion of the experiment, the autoexecute will continue with a pause of 10 minutes. This experiment and pause sequence will now be executed seven more times.



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## Addendum

### Quick PowerSuite-Potentiostat CV test experiment

In this addendum, a quick test procedure is described to setup a simple CV experiment on the potentiostat's internal dummy cell. This test procedure will help you to get started with PowerSuite, as well as to setup an experiment to test the response of your potentiostat.

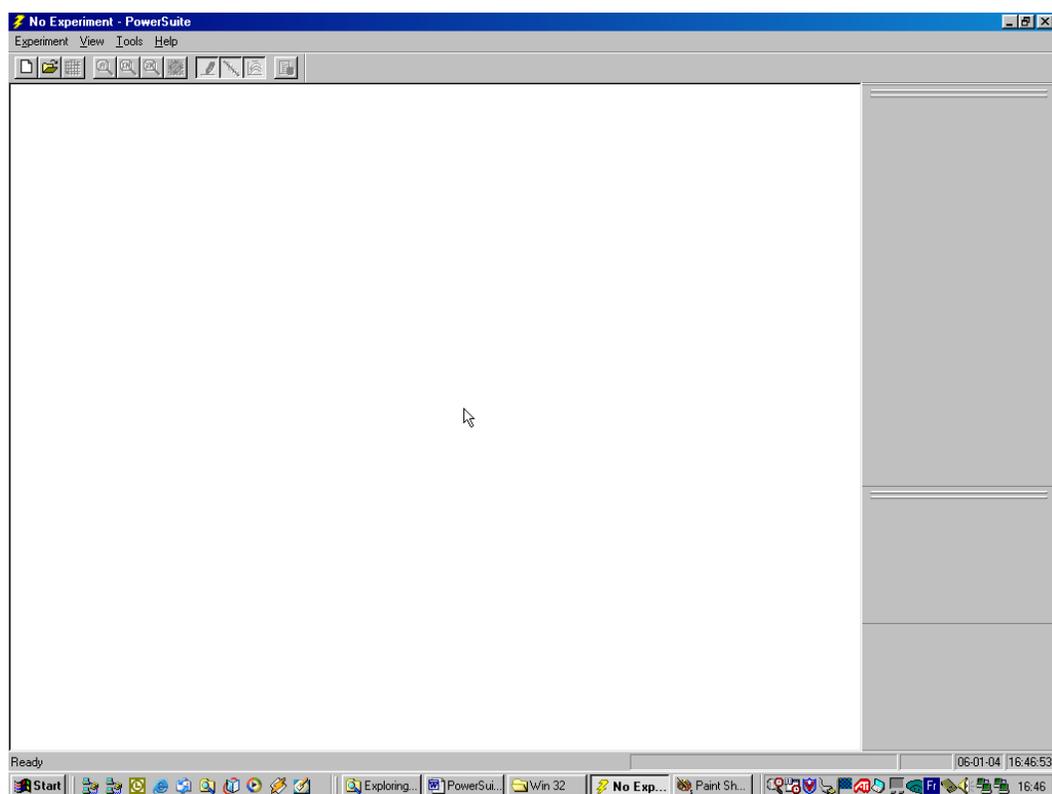
The example described in this addendum will show figures from a PARSTAT 2263-2 potentiostat. It will be quite similar to other types of potentiostats.

The Cyclic Voltammetry experiment has the following setup conditions:

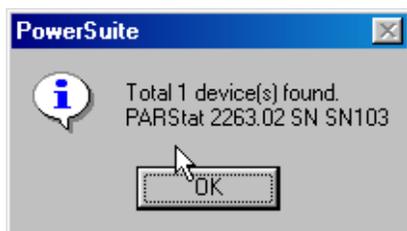
Initial Potential: 0V  
Vertex Potential: +1V  
Final Potential: -1V  
Scan Rate: 100mV/sec

On the internal DC dummy cell of the PARSTAT 2263 (a 1 K $\Omega$  resistor), the current measured at 1V should be 1mA. The CV should show a clean, linear behavior with a perfect overlay of the forward and reverse scans.

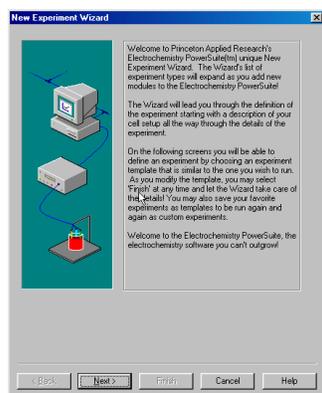
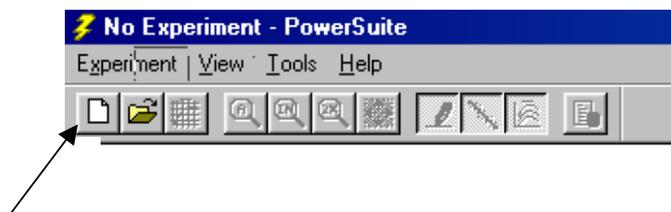
After installing PowerCV 2.40, you should start the experiment with a clean screen. Upon first installation, some sample data will be loaded automatically. Click on « **Experiment** », « **Close** ». You should now have a clean starting page, as follows:



First, you need to make sure PowerSuite is communicating with your potentiostat. Click on « **Tools** », « **Search for Instruments** ». Automatically, a connection window should appear. It should look like the figure below, but the device listed will depend on the type of potentiostat you are working with.

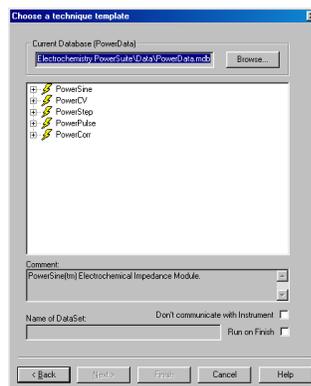


Now let's setup the CV experiment. Click on the « **New** » button to start the **New Experiment Wizard**.

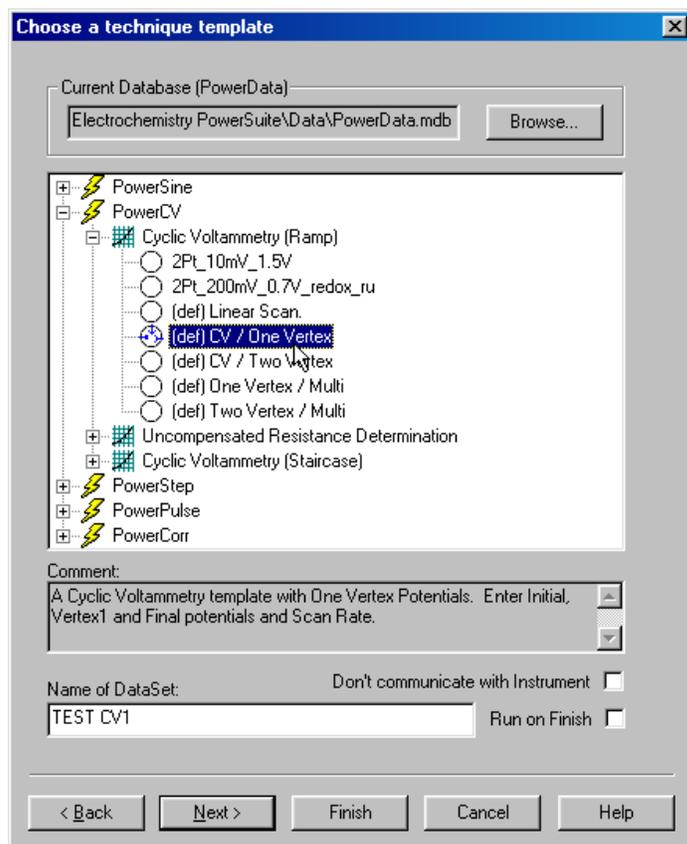


The widow to the left is the Welcome to the New Experiment Wizard Page.

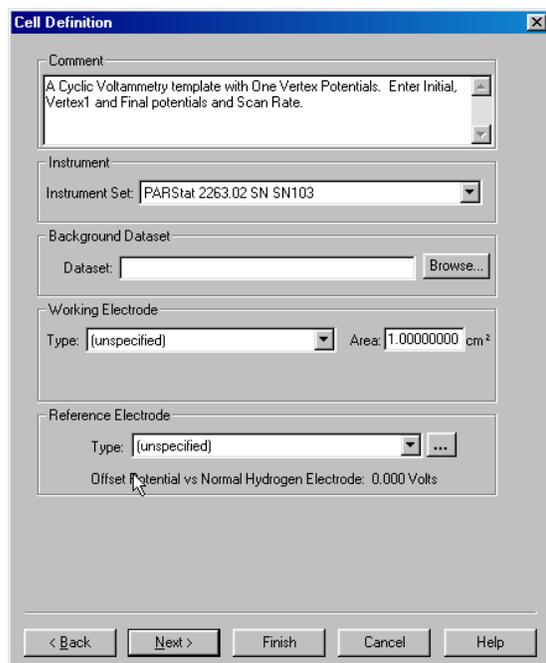
Click « **Next** » to move to the Choose a technique template page (shown at right).



Click on the + sign before **PowerCV**, then the + sign before **Cyclic Voltammetry (Ramp)**. Click on **(def) CV / One Vertex**. Under **Name of DataSet**, type in the test experiment name (in this example « TEST CV1 »). Your screen should look as follows:

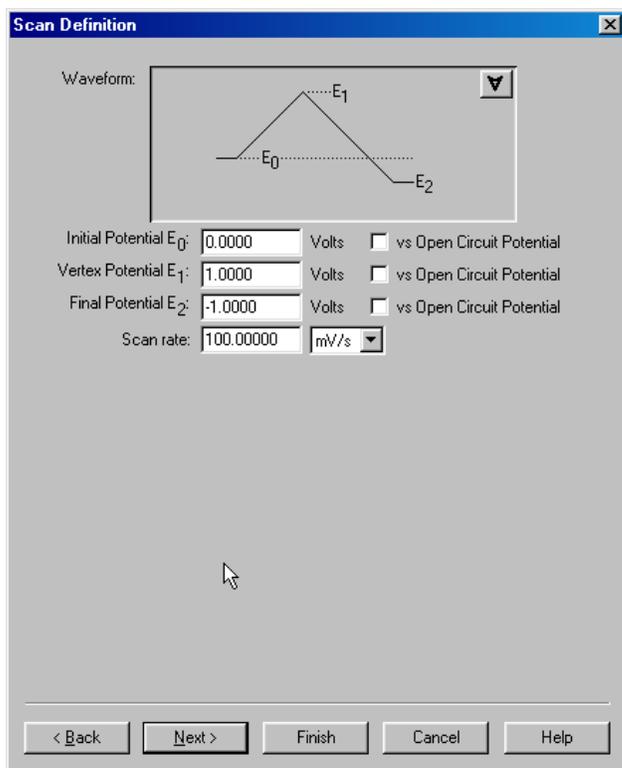


Click on « **Next** » and the **Cell Definition** page should open.

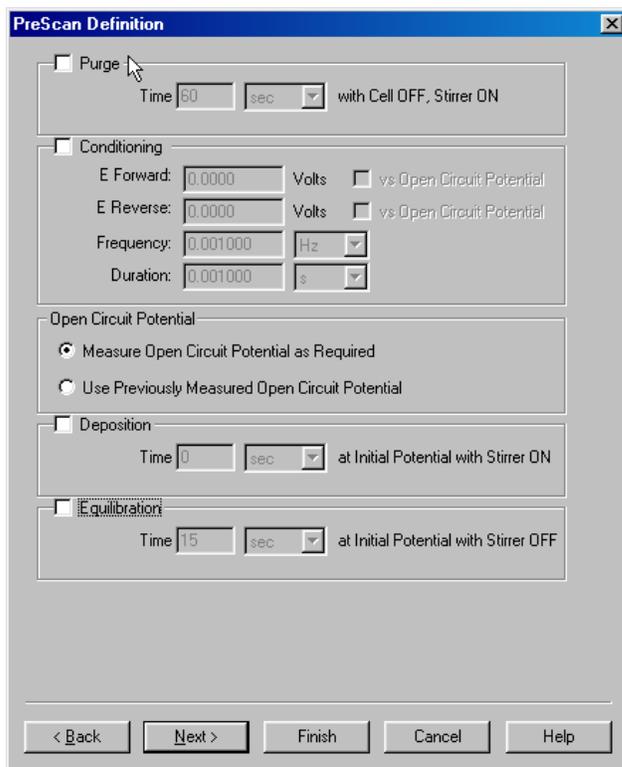


For now, we will not make any changes to the contents. Just make sure that your potentiostat is listed in the **Instrument Set** box. Setting it to **AUTO** will work as well.

Click on « **Next** »



Change the values for the settings as in the example above and click « **Next** » again.

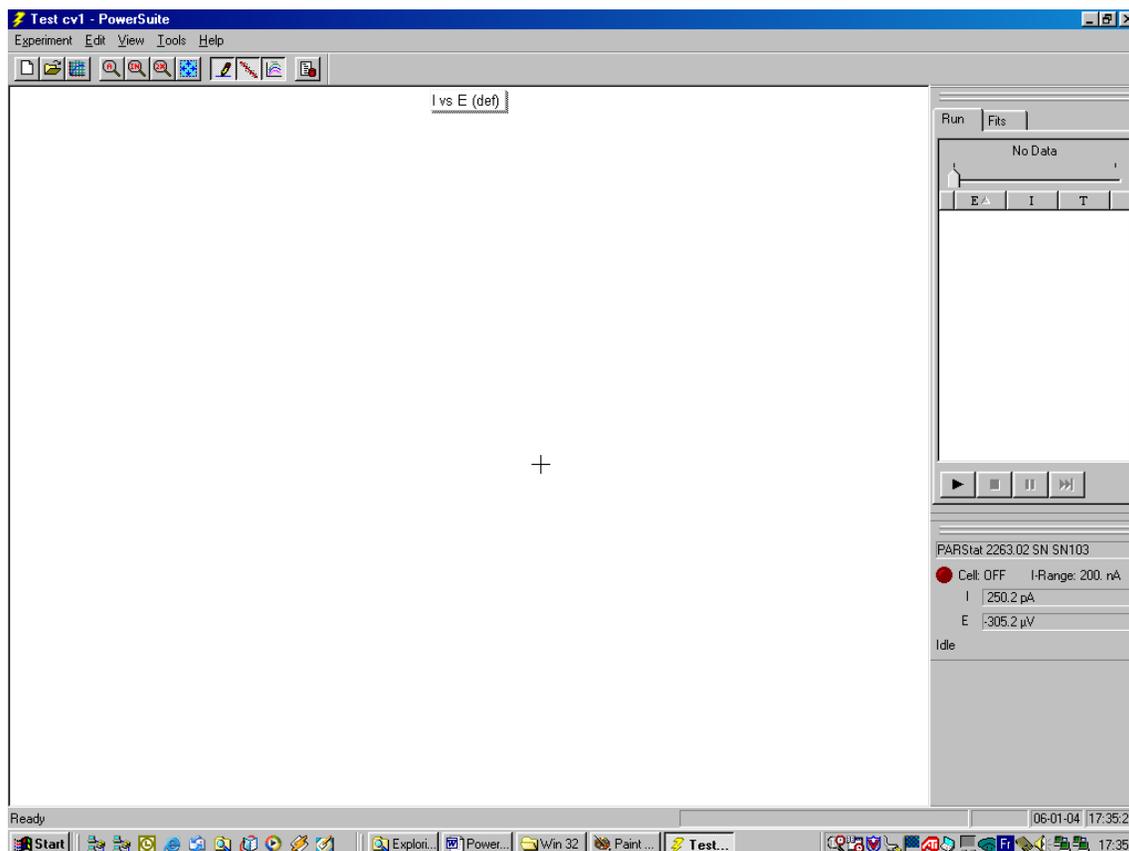


Uncheck the « **Purge** » and « **Equilibration** » functions.

Click on « **Finish** ».

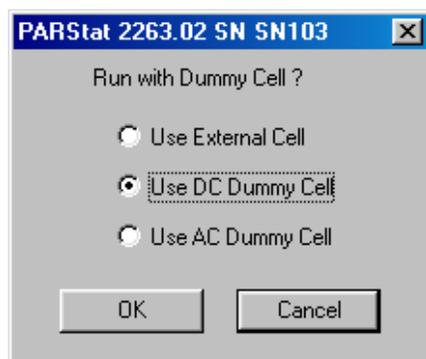
Right away, your potentiostat will be loaded with the proper experimental settings and the instrument bar window (bottom right of the screen) should show the message « **Booting Pstat x%** ». Wait until 100% is reached.

The following screen should now appear. Notice the status of the cell and direct current and potential readings in the instrument bar window.



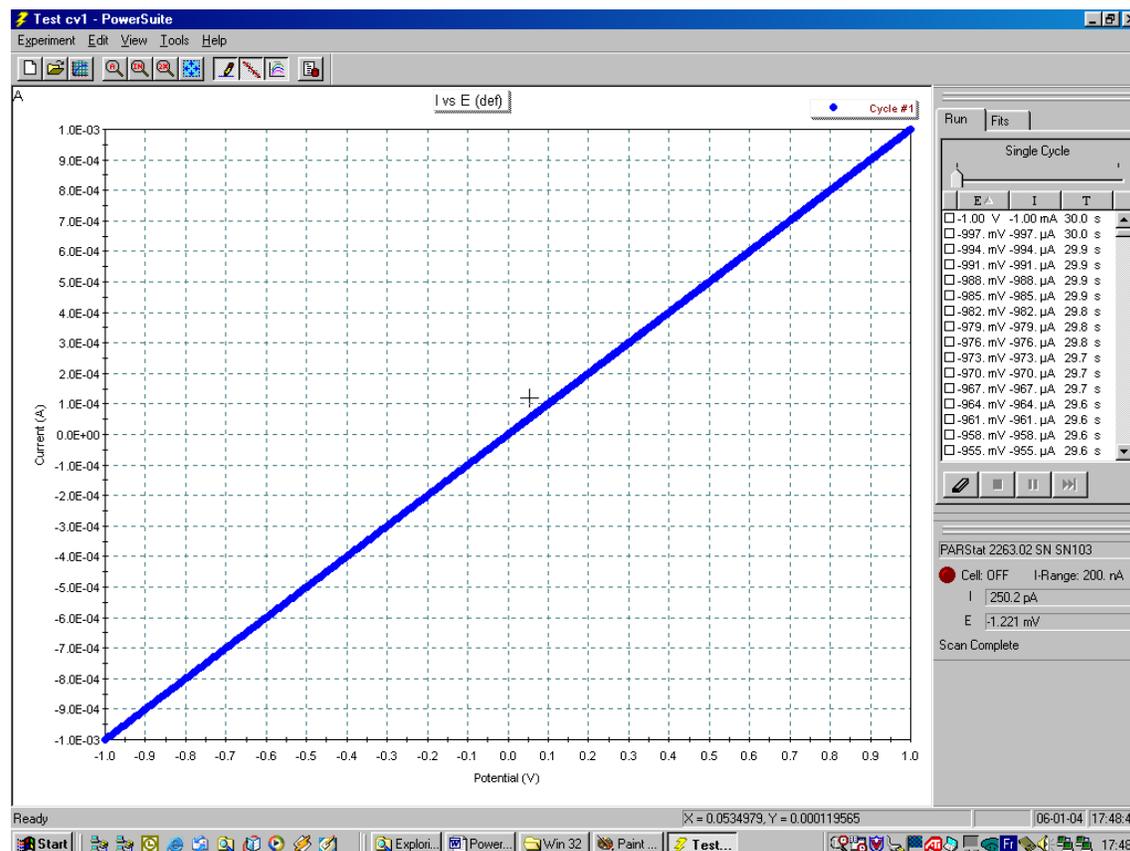
Now click on the « **Run** » button (arrow) to start the CV experiment.

Before continuing, the software will request you to run the experiment on the internal DC Dummy Cell, the internal AC Dummy Cell or the external cell. The following window will appear:

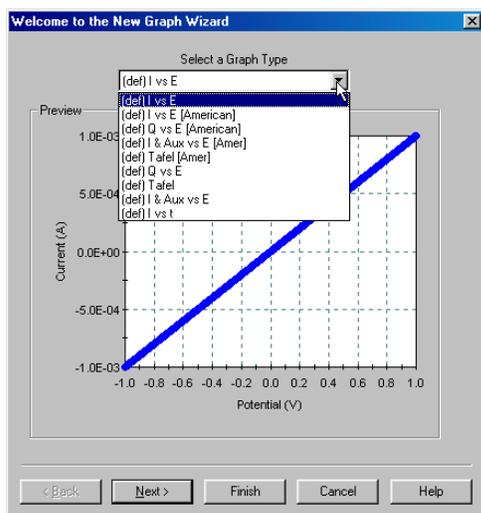


Select « **Use DC Dummy Cell** » and click on « **OK** ». Now your experiment will start and the data will show up in real time on the CV graph.

The experiment will only last approximately 30 seconds (3V scanned with 100mV/s).  
 At the end of the test the results should appear as follows:

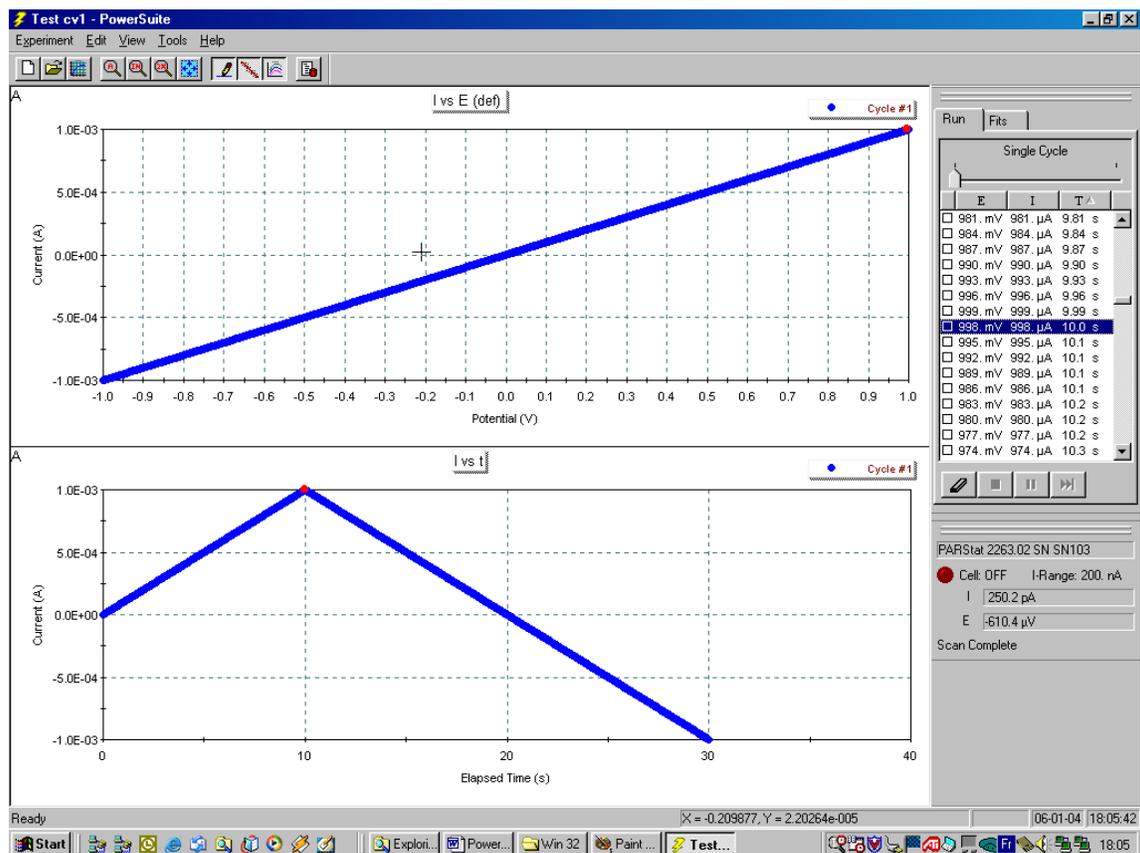


If you want to add another graph to this view, for example Current vs. Time, click on « View », « Add New Graph » and the New Graph Wizard will start up.



Click on the **Select a Graph Type** drop down menu and choose **(def) I vs. t**. Automatically, the graph in the window will change to the new choice. If you want to make changes to the graph setup, you should click « **Next** ». To leave the graph as is, click on « **Finish** ».

The next screen should show both the **I vs. E** and **I vs. t** graphs.



Click on the **T** tab to list all your data as a function of time. Scroll through the data list to find the point at 10 sec and select it by clicking on it. Notice that this selected data point shows up in both graphs as a red highlighted data point.

If your potentiostat is functioning properly, the reading of this data point should give you 1mA +/- 2 $\mu$ A.

This concludes the test phase.

### Quickly exporting your data into Excel

Right Hand click on the graph you want to export, click on « **Copy Data and Graph** ». Start the Excel software, click on « **Paste** » to paste the ASCII data, then click on « **Paste Special** » and select « **Figure** » to paste the graph. In order to copy the full setup conditions into the report, go back into PowerSuite and click on the « **Properties** » button. Click « **Copy** » on the left bottom side of the window. Go back to your spreadsheet and click on « **Paste** ».

An example report is shown below.

