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ZSimpWin Version 3.20

For Windows 95/98/NT/2000/Me/XP

Electrochemical Impedance Spectroscopy

Data Analysis Software

USER MANUAL

the third edition

February 15, 2004

written by

Bruno Yeum, Ph.D.

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ZSimpWin Help Contents

Preface to Version 2.00

Electrochemical Impedance Spectroscopy (EIS) data analysis basically is the determination of optimum parameters associated with a model providing the least deviation of calculated curve from measured data. In principle, selection of a model is sufficient to define a problem. However, computation must start with certain values of the parameters and proceed by applying an optimization method. Estimated solution depends on the values of the parameters. The desired solution is the one associated with the least deviation and can be obtained by trying a large number of combinations, comparing the deviations, and then selecting the one providing the least deviation. For a complex problem, however, the number of trials is too large to be manageable.

The author experienced a lot of frustrations in analyzing data using complex models. With current commercial software in the market, only highly skilled professionals can perform data analysis. They examine data and reduce the number of trials. Satisfactory results are obtained only when the trial values are adequate. For a complex model, determination of these values becomes an extremely difficult task.

The fundamental problem is the requirement of data entry for these trials. Development of ZSimpWin started with the idea of utilizing the high-speed of recent computers for these trials. How about asking a computer to try thousands or millions of combinations and to deliver desired results? In practice, the number of trials had to be drastically reduced by imposing various constraints.

It took the author about 10 months to develop a program which had the intelligence to Autostart (with no other input from the user) and improve the results successively until satisfactory results were obtained. The author presented this work to Princeton Applied Research in April, 2000. Princeton Applied Research's personnel were excited about these results and provided assistance for further improvements.

This version was satisfactory in producing desired results, however, required substantial enhancements in graphics and data management to meet the high standards of recent Windows-based applications. In the last 8 months, the author continuously changed the appearance, added more features, reorganized functions, and minimized the number of mouse button clicks by combining a sequence of operations.

In the last couple of months, the author devoted much time to implement automatic saving of computational results. Now data analysis process is very simple with ZSimpWin. The user defines a job by specifying a data file and selecting a model, and then requests its execution. ZSimpWin takes over all the complex operations. It autostarts, performs computations a number of times to determine the desired solution, and saves these results. When data analysis is finished, the user examines these results and prepares reports.

The ZSimpWin has been created to make EIS data analysis fun and easy. You will enjoy the adventure of data analysis with ZSimpWin.

Bruno Yeum, Ph.D.
Echem Software
Ann Arbor, Michigan, USA

February 2001

Upgrades from V2.00 to V3.00

After the release of ZSimpWin Version 2.00, we have been anxious to hear from you about its operation in various environments. Based on your critical comments and suggestions, we could locate the following areas requiring improvements:

1. Sometimes, ZSimpWin seems to keep on running in iterate mode without changing any parameters.
2. Can we create a list of the items to be printed and print these items in sequence?
3. The plot pasted to a document and corresponding printed plot look different.
4. It is convenient to prepare a report as a file because it can be distributed as an email attachment. Can we reduce the number of the steps required to prepare a report?
5. In simulate mode, it is desirable to view the input parameters and corresponding plot on a screen.
6. In European countries, commas are used as decimal separators for floating numbers. EIS data with commas are not accepted in Version 2.00.
7. Created an Input Folder and stored impedance data, however, ZSimpWin refused to save computational results because matching Output folder had not been created. How about letting ZSimpWin to create the Output folder if it does not exist?
8. Want to read the coordinate of a data point especially in the complex plane plots (Nyquist, Admittance, and Capacitance).

In addition to making improvements in these areas, we have added many other useful features. See **"Upgrades from V 2.00 to V 3.00.doc"**. You will find that this version provides much higher efficiency in data analysis and document preparation.

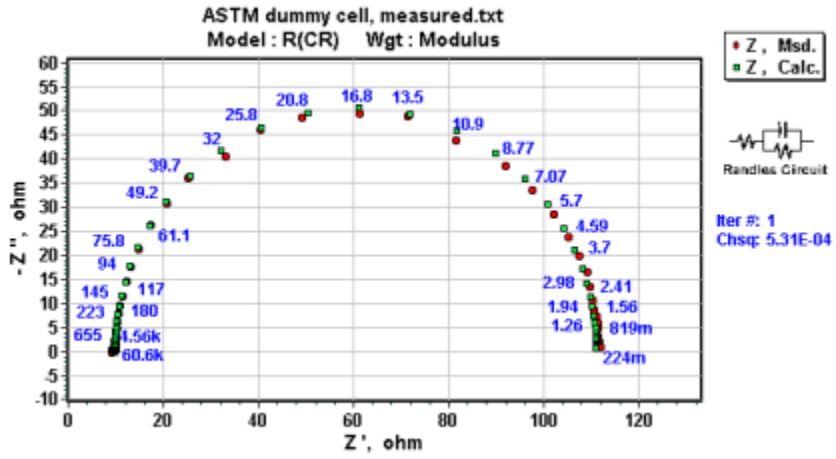
Thank you for your support and assistance.

Bruno Yeum, Ph.D.
Echem Software
Ann Arbor, Michigan, USA

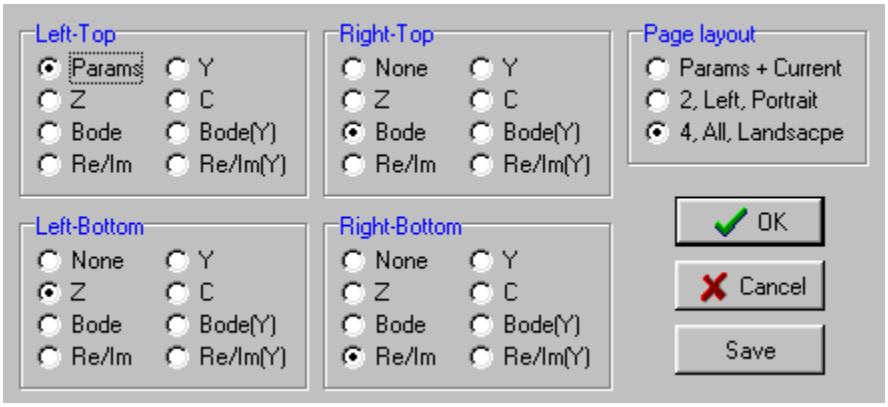
January 2002

More features in V3.20

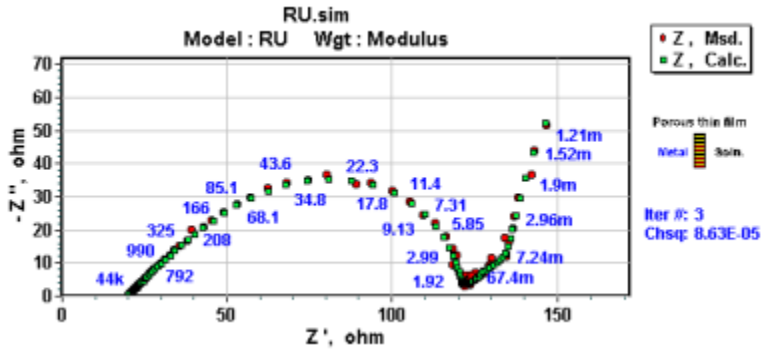
- Displays frequency labels on complex plane plots (Nyquist, Admittance and Capacitance).



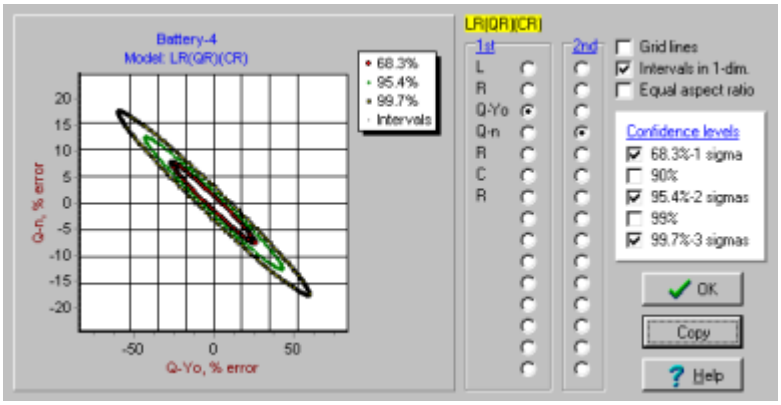
- More flexible selection of print items - Two items in portrait orientation or four items in landscape orientation.



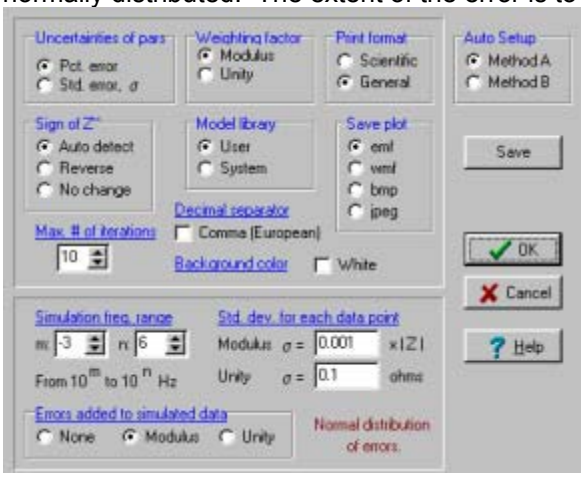
- Additional circuit elements associated with porous electrodes and diffusion problems - Demonstrates the capability of fitting data to a well-defined impedance expression by adding a circuit element (See Extended circuit elements)



- Displays confidence regions in two parameters - Based on calculated covariance matrix.



- Errors can be included in simulated data - The error for each data point is assumed to be normally distributed. The extent of the error is to be specified in the Options dialog box.



Next topic: What is ZSimpWin?

What is ZSimpWin?

ZSimpWin is an Electrochemical Impedance Spectroscopy (EIS) Data Analysis Software utilizing the fast computation speed of recent computers. Innovative concepts have been implemented to achieve the following performance:

1. MInimal user input: The user specifies a job by selecting a model for an impedance data set, and simply requests execution to ZSimpWin.

2. Automatic analysis: Parameters associated with the selected model are determined automatically. ZSimpWin assigns an initial guess of these parameters (default: Auto Setup option), starts computation using the initial guess, finds results, improves these results a number of times until desired results are obtained, and then saves the final results.

3. Processing multiple jobs: Setup a batch by including multiple jobs, and process in sequence. Analysis results are saved in a designated folder.

4. Output results in various forms: Analysis results consist of plots, estimated parameters, and historical records of computation process. Each or several combinations can be printed or copied to Windows clipboard. The most convenient form is printing estimated parameters and displayed plot on a single page.

5. Requires only mouse button clicks: The whole process requires no entry of numbers or character strings. Only mouse button clicks are required.

See also:

- Main Features.
- ZSimpWin Main Window.

Introduction

This section describes the application of Nonlinear Least Squares Fit principles to analyze electrochemical impedance spectroscopy data and the problems encountered in the determination of optimum parameters.

Optimization Principles
Definition of the chi-squared
Problem Statement
Implementation
Down-hill simplex Method

Next topic: Optimization Principles

Optimization Principles

- Model electrode kinetics with an equivalent circuit consisting of electrical components.
- Define a merit function (called χ^2) with the parameters in the model, measured data points, and the standard deviations of the data points.
- Assume a certain behavior of the standard deviations (Weighting).
- Determine the parameters providing the global minimum of the function.

Next topic : Definition of the Chi-squared

Definition of the Chi-squared

The parameters providing the best fit to a model is obtained by minimizing the function (χ^2) defined as the sum of the squares of the residuals.

Data points and parameters

1. Experimental data point (frequency, Z real, Z imag)

$$[\omega_i, a_i, b_i]$$

2. Parameters associated with a model

$$\vec{p} = (p_1, p_2, p_3, \cdots p_m)$$

3. Calculated point

$$[\omega_i, Z'(\omega_i; \vec{p}), Z''(\omega_i; \vec{p})]$$

4. Weighting factors

$$[\omega_i, W_i', W_i'']$$

Application of statistics

The distance between exp. and cal. Points

$$d_i^2 = (a_i - Z'(\omega_i; \vec{p}))^2 + (b_i - Z''(\omega_i; \vec{p}))^2$$

The goodness of fit to model

$$\chi^2 = \sum_{i=1}^{n} \frac{\left[(a_i - Z'(\omega_i; \vec{p}))^2 + (b_i - Z''(\omega_i; \vec{p}))^2\right]}{\sigma_i^2}$$

where *n* is the number of data points.

Weighting Options

Unity weighting $\sigma_i = f$

Modulus weighting $\sigma_i = f\sqrt{a_i^2 + b_i^2}$

Next topic : Problem Statement

Problem Statement

We are looking for the global minimum of the χ^2 defined as a function of ***n*** parameters. For a large value of ***n*** (e.g., 10), this function is most likely to have multiple minima, and determination of this minimum becomes a formidable task.

A gradient method is often employed for optimization. Computation starts with an initial guess. A local minimum is readily obtained, however, this local minimum is most likely to be different from the global minimum.

Fundamental problem is difficulty of finding an adequate initial guess.

Many trials are required to find an adequate initial guess leading to the global minimum. Highly skilled professionals apply basic principles to substantially reduce the number of the trials by estimating some of these parameters. However, it can be extremely difficult to find an initial guess leading to the global minimum especially for a large number of parameters.

Next topic: Implementation

Implementation

The innovative feature of ZSimpWin is elimination of the initial guess. ZSimpWin keeps on finding a local minimum after each iteration until the global minimum is found. See the Flowchart: Running in Iterate Mode. ZSimpWin starts with a rough initial guess, i.e., the start point of the 0th iteration, arbitrarily selected by ZSimpWin (Auto Setup). When a local minimum is found, the best start point for the next iteration is searched based on the local minimum and the values of the estimated parameters. This start point leads to another local minimum lower than the one found in the previous iteration. This iterative steps are repeated until the global minimum is found. The end of the iteration is characterized by no success in finding a local minimum lower than the previous one. This local minimum is equal to the global minimum.

Next topic : Down-hill Simplex Method

Downhill Simplex Method

ZSimpWin employs downhill simplex method for function optimization.

Problems with gradient methods (e.g., Marquardt Method)

- Derivative calculation and matrix algebra
- Numerical overflow ("Matrix singularity error" due to ill-conditioned matrix).
- Not easy to impose various types of constraints

An extensive search requires trying with combinations of the values of the parameters each of which varying by many orders of magnitudes. Matrix algebra would fail when any of these parameters have negligible effect on the function to be minimized (χ^2).

Down-hill simplex method

This method is basically a **trial-and-error** method. A function is evaluated at assigned trial points and compared to each other. Based on the values at these points, the next trial points are intelligently determined. Function evaluations and comparisons are repeated until a local minimum is reached. This method was adopted because of the following characteristics:

- No derivative calculation and no matrix algebra
- Simple and robust.
- Easy to impose constraints

Next topic: Equivalent circuit

Equivalent circuit

This section describes the definitions and symbols of circuit elements, modeling electrochemical impedance data with an equivalent electrical circuit, and guideline to select most probable models representing the impedance data.

- **List of Standard Circuit Elements**
- **Circuit Description Code**
- **Extended circuit elements**
- **Description of extended circuit elements**
- **Testing extended circuit elements**
- **Show tips**

List of Standard Circuit Elements

Elements, corresponding symbols, and parameters are listed below:

Description	Symbol	Parameters	Admittance
Resistance	*R*	*R*	$1/R$
Capacitance	*C*	*C*	$j\omega C$
Inductance	*L*	*L*	$-j/\omega L$
Warburg	*W*	Y_0	$Y_0\sqrt{j\omega}$
CPE	*Q*	Y_0, n	$Y_0(j\omega)^n$
Tanhyperbolic	*T*	Y_0, B	$Y_0\sqrt{j\omega}\tanh\left(B\sqrt{j\omega}\right)$
Cothyperbolic	*O*	Y_0, B	$Y_0\sqrt{j\omega}\coth\left(B\sqrt{j\omega}\right)$
Gerischer	*G*	Y_0, K_a	$Y_0\sqrt{K_a + j\omega}$
Havriliak-Negami	*H*	$(C_0 - C_\infty), \tau_0, \mu, \phi$	$j\omega(C_0 - C_\infty)\left[1+(j\omega\tau_0)^\mu\right]^{-\phi}$

Circuit Description Code

Boukamp used an intelligent method of representing an equivalent circuit. See Equivalent Circuit Users Manual for detailed description. Circuit Description Code (CDC) consists of element symbols nested by parentheses of several levels.

Sample code: L1 R2 (C3 (W4 (R5 C6)))

Definitions

- **Simple element** : independent (R, C, L, W, Q, T, O and G). See List of circuit elements for the meaning of these symbols.
- **Complex element** : series or parallel circuit containing simple and/or complex elements of higher order
- **Order of a complex element** : the number of boxes containing the element including its own box.

Assignment of the order

- Start with order zero (ground level). Several elements or no element may be present at the level.
- Raise the order when left parenthesis is encountered.
- Lower the order when right parenthesis is encountered.
- The number of left and right parenthesis should be equal in a valid code.

The items enclosed by matching left and right parentheses are included in a complex element.

Element L1 R2 (Q3 (W4 (C5 R6)))
Order 0 0 1 2 3 3 2 1 0

Recursive definition of complex element
Complex elements are divided into alternating series/parallel arrangements of simple and complex elements of increasing order, until only simple elements remain.

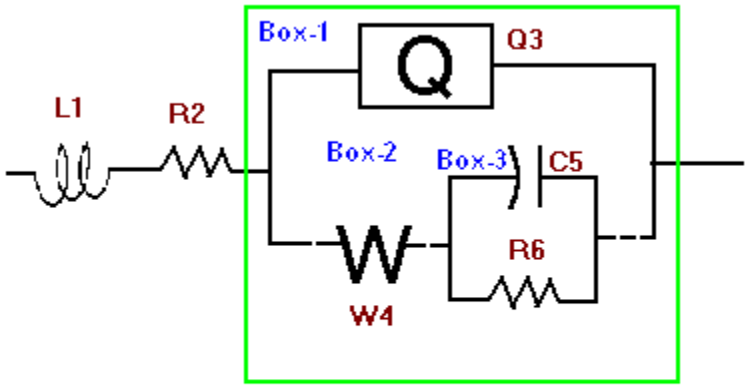
Alternation rule

- A complex element is represented either
  by simple elements of order (n-1) and a complex element of order n, i.e., A (Box-n), or
  by simple elements of order n, i.e., A B.

- A and (Box-n) are in series if (n-1) = even, and in parallel if (n-1) = odd. Simple elements are in series if n = even, and in parallel if n = odd.

Orders	Structure	Series or parallel
0, 1	L1R2 (Box-1)	L1R2, (Box-1) in series
1, 2	Q3 (Box-2)	Q3, (Box-2) in parallel
2, 3	W4 (Box-3)	W4, (Box-3) in series
3, 3	C5 R6	C5, R6 in parallel

Equivalent circuit represented by the sample code



Reference : B.A. Boukamp: EQUIVALENT CIRCUIT Users Manual, second edition, 1989.

Extended circuit elements

This feature has been added in the **V 3.20** release.

Even though a simple impedance expression is available, it might not be represented with an equivalent circuit. To find the optimum values of the parameters associated with this expression, we can create a new circuit element.

This Note gives a brief description of the circuit elements created to represent unique impedance expressions. The assumption and approximations involved in deriving these equations are not fully listed. Consult the references for details.

In principle, any well-defined impedance expressions can be handled. However, the parameters associated with this equation might not be obtained by running ZSimpWin in Iterate Mode. This problem is most likely to be caused by:

No unique solution : When different combinations of parameters lead to the same impedance, multiple roots exist. It might not be possible to find one of the roots.

Inadequate initial guess: Might lead to numerical overflow if selected initial guess is not adequate.

Large uncertainties of parameters: The number of parameters defining the impedance is more likely to be larger (typical values are 2 to 6) than that for standard elements. When experimental data do not reflect the unique effects of each of the parameters, it would be more difficult to separate these effects.

If you are interested in fitting your data to your own formula, we might be able to create a circuit element for you. Show us your impedance expression and provide a couple of sample data.

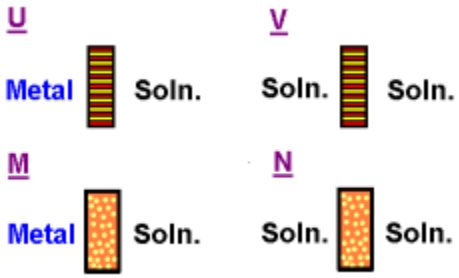
Next topic: Description of extended circuit

Description of extended circuit elements

Circuit symbols were arbitrarily assigned to the impedance expressions derived based on simple models for the following physical phenomena:

Macroscopically homogeneous porous electrodes (Circuit symbol = U, V, M, or N)

- Applied transmission line models (TLM).
- Solutions of partial differential equations for the potential distributions in the solid and the liquid phases under different boundary conditions.
- Local impedance was derived based on linear coordinates.



U = Metal-film-solution. Asymmetric boundary conditions. Ohmic current at the metal-film side. Ionic current at the film-solution side. Cylindrical pores.

V = Solution-film-solution. Symmetric boundary conditions. Ionic currents at both sides. No ohmic current. Cylindrical pores.

M and N: Local impedance was derived based on spherical coordinates (spherical pores of uniform size).

Simple model for electrochemical capacitors (Circuit symbol = P)

- The resistance of the bulk material is much smaller than the electrolyte resistance.
- Straight cylindrical pores.

Capacitance drops sharply above a characteristic frequency.

Havriliak-Negami element (Circuit symbol = H)

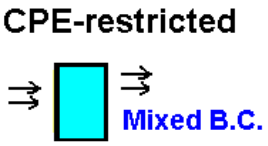
Empirical relation for dielectric constant includes the special cases of Davidson-Cole response (skewed arc) and ZARC-Cole (depressed semicircle).

Bode, Real/Imag, and Admittance plots can be taken based on impedance or capacitance. For dielectric systems, we want to display these plots in capacitance.

Select the dielectric system by clicking on the **Dielectric | Dielectric system** menu.

Linear Diffusion (Circuit symbol = B)

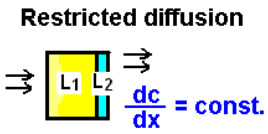
- Single layer. CPE-restricted.
- General expression of linear diffusion regardless of various boundary conditions.



Includes the limiting cases:
- Restricted.(α=1) : Constant concentration gradient (flux).
- Bounded (α=0) : Constant concentration.

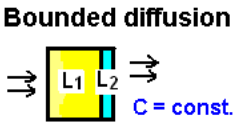
Bilayer, Restricted diffusion (Circuit symbol = I)

When the thickness of the second layer is very small, this case becomes the limiting case of the restricted boundary condition for a single layer.



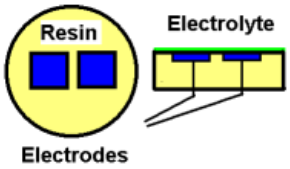
Bilayer, Bounded diffusion (Circuit symbol = J)

When the thickness of the second layer is very small, this case becomes the limiting case of the bounded boundary condition for a single layer.



Axial diffusion through a film (Circuit symbol = X)

- A pair of identical electrodes are covered with a thin electrolyte layer.
- Impedance was derived for a unique electrode configuration.
- Transmission line model (TLM).

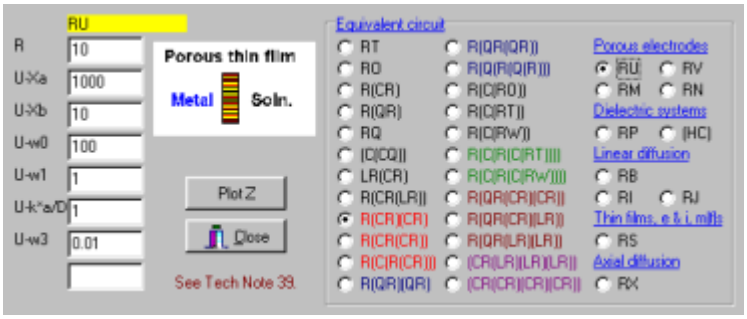


Next topic: Testing extended circuit elements

Testing extended circuit elements

An equivalent circuit containing an extended element should lead to proper impedance. It is also necessary to be able to get the least-squares fit in **Iterate Mode**.

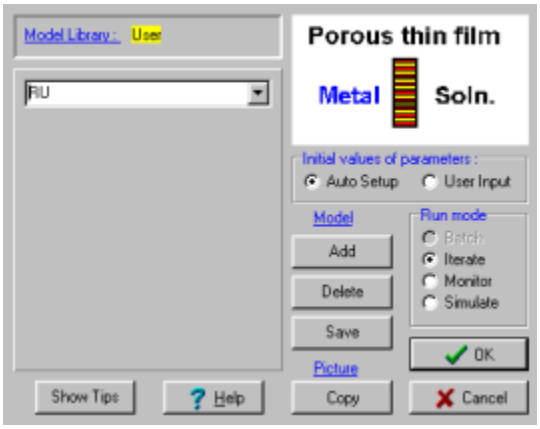
1) Select an equivalent circuit and run in **Simulate Mode**. Enter the values of the parameters.



2) Check whether calculated data represent the impedance.

3) Save impedance data (**File | Save Impedance Data**). The data will be saved as **…\data\simulation data*.sim**, and then automatically taken as input data.

4) Run in **Iterate Mode** to fit the data to the same circuit. Click on the **[OK]** button.



This test has been performed with very good data and starting with a good initial guess. It might be necessary to change the initial guess for other data (Run in **Iterate Mode** with the **User Input option**).

Next topic: Show tips

ZSimpWin Overview

System Requirements
Installation
ZSimpWin Main Window
Main Features

Quick Start

Models in System Library
Printing User Manual

Next topic: System Requirements

System Requirements

ZSimpWin will run on any IBM PC or compatible computer that supports Windows 95, Windows 98, Windows NT, Windows 2000, Windows Me, or Windows XP. Because ZSimpWin requires a lot of computational efforts, it is recommended to use a high speed (at least 350 MHz) Pentium microprocessor for best results. Additional requirements are:

- A minimum of 128 megabytes of memory (RAM).
- A VGA display of 800x600 is recommended.
- A Windows-supported mouse.

Next topic: Installation

Installation

ZSimpWin is installed to the folder, **C:\Program Files\ZSimpWin**, as default. Another folder can be selected at the installation stage. This folder is the **Application folder**.

If you are upgrading from an old version (2.00, 2.10, 3.00, or 3.10),

1. Uninstall the old version.
2. Delete the registration key file in the **Application Folder**.
3. Install the new version.

ZSimpWin is supplied on CD-ROM.

1. Insert the disk in the CD-ROM drive.

2. Double click **My computer** on the Desktop.

3. Double click **CD-ROM** Drive ("D:", "E:", or "F:" depending on your system).

4. Double click **Disk1** folder.

5. Find  and double click to start installation.

6. Answer the installation wizard prompts and click on the **[Next]** button.

Uninstall

If a Demo version or a previous version is installed in your computer, remove this version following Windows standard uninstall procedure.

1. Click **My Computer**.
2. Click **Control Panel**.
3. Click **Add/Remove Programs**.
4. Select **ZSimpWin** to remove.
5. Click on the **[Add/Remove]** button.
The "Confirm File Deletion" dialog box will appear on the screen. You will get the message, "Are you sure you want to completely remove the selected application and all its components?"
6. Click on the **[OK]** button.

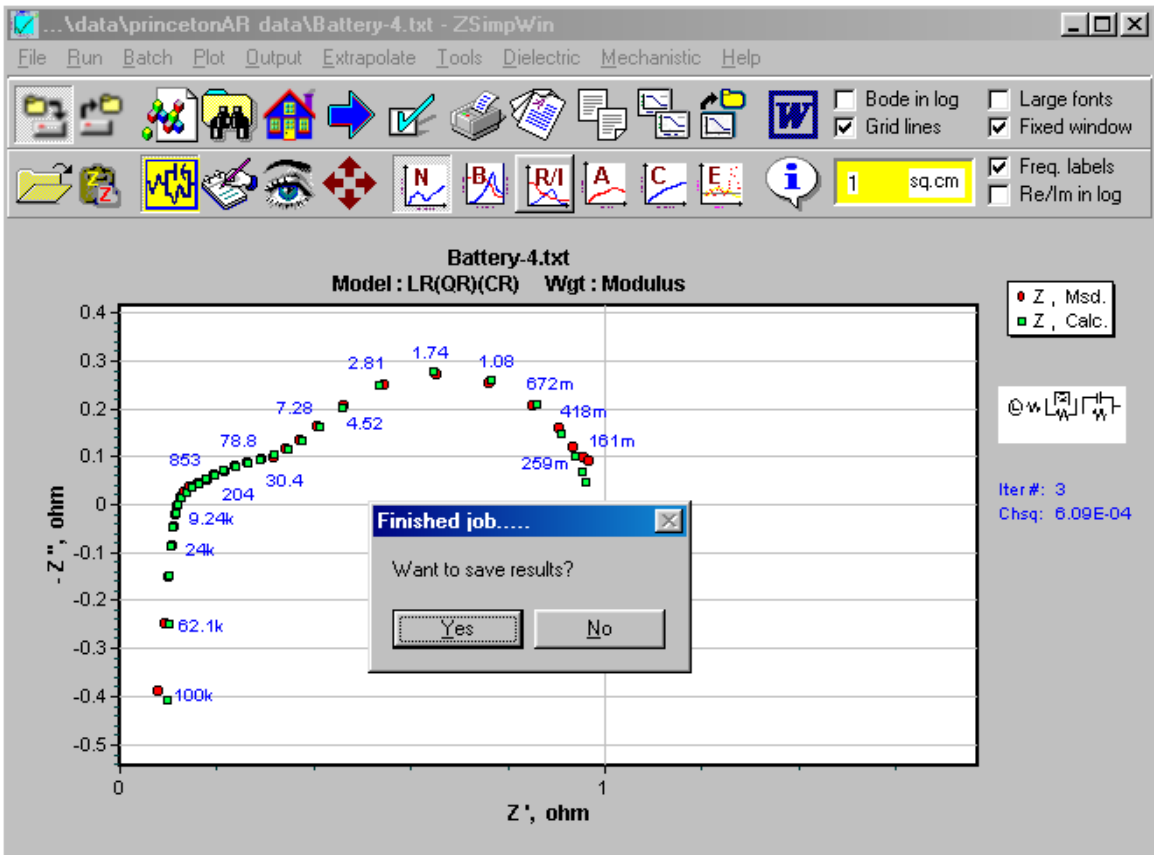
Note that all the folders and the files copied during installation of the old version would be completely removed. However, the files you copied for your work or testing would not be removed.

Next topic: ZSimpWin Main Window

ZSimpWin Main Window

This is the main window of the ZSimpWin. In this window you'll be able to see most of the functions by clicking on the main menus or speed buttons in the tool bars.

This is the image indicating the presence of hot spots in the picture.



Next topic: Main features

File Menu

Open...
Paste Z Data

Retrieve Parameters
Save Parameters

Save Impedance Data
Save Converted (C or Z Data)
Delete Selected Point

Exit

Run Menu
Select Model &Run Mode
Edit Parameters & Run
View, Print & Copy Results.
Options

Run in Simulate Mode
Convert CPEs to Capacitors

Plot Menu
Nyquist
Bode
Real/Imag
Admittance
Capacitance
Errors
Bode(Y)
Real/Imag(Y)

Bode in Logarithm
Show Grid Lines
Use Large Fonts
Fixed Window
Freq. Labels
Re/Im in Logarithm

Batch Menu
Setup & Process
Locate Results
Go Home
Move to Next
Check Progress

Extrapolate Menu
Apply Kramers-Kronig
Add Points
Remove Points
Calculate Impedance
Save Extrapolated Curves

Output Menu
Print Item Selection
Print Project Groupt
Copy Results
Copy Plot
Save Plot

MS Word Document

Dielectric Menu
Conductive System
Dielectric System

Read Z Data
Read C Data

Tools Menu
Export Data
Enter Sample Area
Create New Folder
Append Header Lines
Get Pseudocapacitance

Change Chart Titles
Edit Sample IDs
Specify Image Viewer
View Saved Plots

Mechanistic Menu
Application of reaction models.

- Simple Passivation Model
- Passivation of Chromium
- Electrocrystallization of Nickel
- Dissolution of Zinc in Sulfate
- Dissolution of Iron in Acid

Help Menu
Contents
How to run
About

Registration
Technical support

Hot spot
A point of reference that provides additional information concerning the picture, word, or group of words on which cursor is resting.

Pop-up Menu
Click the right mouse button to access the pop-up menu. Most of the menu items in the main menu can be selected from this menu.

Nyquist plot
Data points are on a complex plane. Displays the real and imaginary components of the impedance in the x- and y- axes, respectively, with each point associated with a frequency.

Bode plot
Displays the absolute value of the impedance and the phase angle as functions of frequency.

Real and Imaginary
Displays the real and imaginary components as functions of frequency.

Admittance plot
Data points are on a complex plane. Displays the real and imaginary components of admittance in the x- and y- axes, respectively, with each point associated with a frequency.

Capacitance plot
Data points are in the complex plane. Displays the real and imaginary components of capacitance in the x- and y- axes, respectively, with each point associated with a frequency.

Error plot
Error for each data point in % error and phase angle.

Bode(Y)
Displays the absolute value of the admittance and the phase angle as functions of frequency.

Real/Imag(Y)
Displays the real and imaginary components of admittance as functions of frequency.

Picture of selected model
Displays the picture associated with selected model.

Chi-squared value
Displays the chi-squared value (associated with its local minimum) after each iteration.

Show Grid Lines
Show grid lines.

Use Large Fonts
Use large fonts for the chart title, axis titles, axis labels, and legends. Uncheck for small fonts. If you want to copy a plot to Windows clipboard and paste to a document, try the large fonts option.

Bode |Z| in Logarithm
Displays a Bode plot in log |Z| vs log (frequency) or |Z| vs. log (frequency).

Fixed Window
ZSimpWin maintains the equal scaling factors of the real and imaginary axes in the Nyquist, Admittance and Capacitance plots. This is achieved by extending the ranges or lengths of the axes. In the former case, the size of the window is fixed. Whereas in the latter case, the size of the window is adjusted depending on the ranges of the axes.

Freq. Labels
Displays the frequency labels in complex plane plots (Nyquist, Admittance and Capacitance).

Re/Im in Logarithm
Displays the real and imaginary components in log scale.

Save simulation
Save simulated results as a parameter file with the model name.

Save Converted (C or Z Data)
The first step is data conversion; impedance data (frequency, Z' and Z") to capacitance data (frequency,

C' and C") or capacitance data to impedance data. The next step would be saving the converted data as a file.

Read Impedance Data
Read data in impedance format (frequency, Z' and Z").

Read Capacitance Data
Read data in capacitance format (frequency, C' and C").

Save Plot
Saves the current plot as a file in EMF, WMF, BMP, or JPG format in the **.../pics/** folder. Select the format from the Options dialog box. A save filename is suggested. This name consists of the input filename, selected model name, and the displayed plot style. The filename extension represents the selected format ("EMF", "WMF", "BMP", or "JPG"). Click on the **[Yes]** button to accept this name. If you click on the **[No]** button, you are requested to enter the filename and select its destination.

MS Word Document
Opens the Microsoft Word document Window to paste copied results or plot.

Specify Image Viewer
Specifies an image viewer installed on the computer. The name of the program and its location are stored. This program will be used to view saved plots in the current and later sessions.

View Saved Plots
Saved plots are viewed using selected image viewer. The image viewer should have been specified previously (See "Tools | Specify Image Viewer").

Convert CPEs to Capacitors
Converts CPEs (Q) in the selected CDC to capacitors and saves the impedance data and corresponding parameters. Computation in Iterate Mode should have been completed with the selected CDC or parameters should have been retrieved.

Get Pseudocapacitance
Computes the equivalent capacitance for a CPE by keeping the relaxation time constant associated with the CPE.

Main Features

ZSimpWin = Automatic start, computation, and saving of results. When impedance data are read and a model is selected, a rough initial guess is assigned by ZSimpWin and then computation starts immediately. The final results are used to determine the initial guess for the next iteration. Successive iterations improve the initial guess as well as the final results.

Main features are listed below:

1. Runs with Windows 95/98/2000/Me/XP.

2. Needs minimal technical expertise to run.

3. No numerical data entry in most occasions.

4. Excellent user interface. Use speed buttons in the main window to access menus.

5. Determines the absolute minimum (true solution) rather than a local minimum (wrong solution).

6. Processing multiple jobs in sequence.

7. Circuit Description Code is used to identify an equivalent electrical circuit.

8. Reads PowerSine, Gamry (*.dta), ZView (*.z, *.z60), and text formats.

9. Presents plots and parameters in various formats.

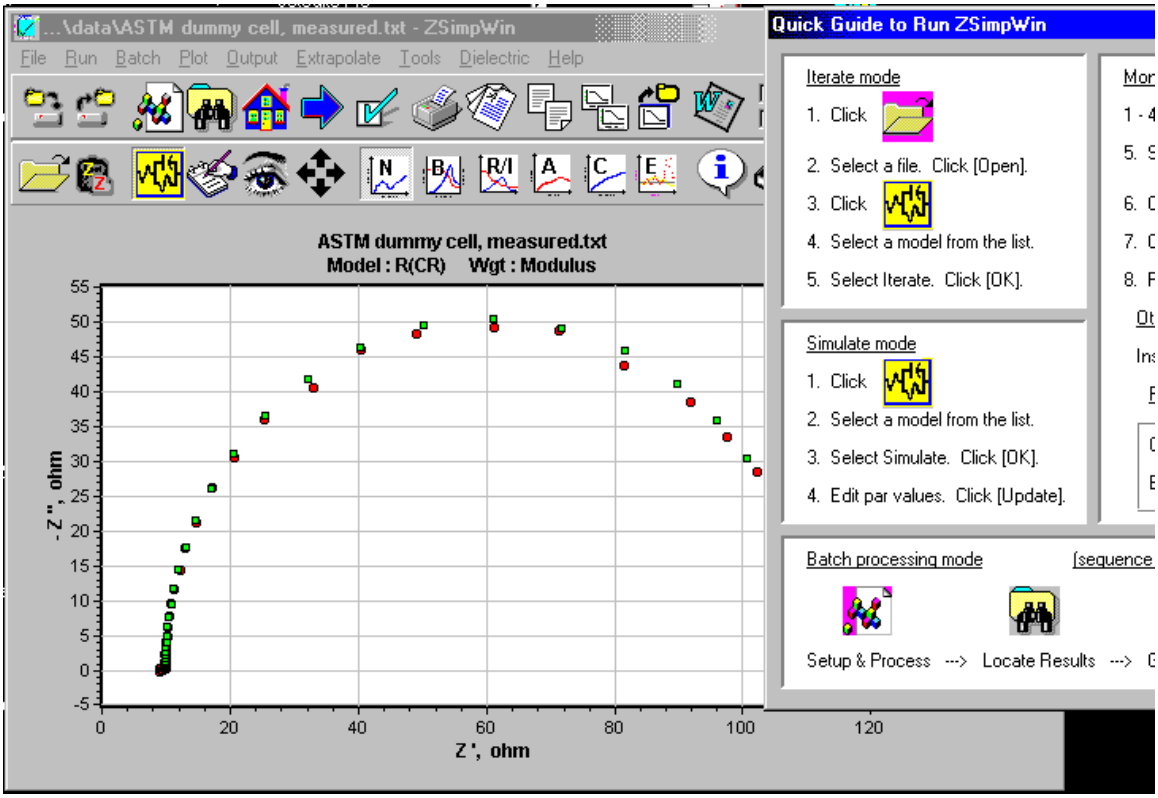
10. Plots and parameters can be copied to Windows clipboard, and then pasted to other document.

11. Can focus an area for close examination (See Close examination of a local area).

12. Can read the coordinate of a data point (See Reading the Coordinate of a Data Point).

Quick Start

1. Click  to show the ~~Quick Guide to Run ZSimpWin~~ dialog box.
2. Move the box to the top-right corner of the screen.
3. Run in **Iterate mode** with sample impedance data.
4. Run in **Simulate mode** (e.g., Model = R(CR), Values = 10, 1e-5, 100).



Next topic: Models in System Library

Models in System Library

The models in the System Library are as follows:

(C(CQ))
(C(R(CR)))
(C(R(LR)))
(C(RW))
(CR(CR)(CR)(CR)(CR))
(CR(CR)(CR)(CR))
(CR(CR)(CR))
(CR(CR))
(CR(LR)(LR)(LR)(LR))
(CR(LR)(LR)(LR))
(CR(LR)(LR))
(CR(LR))
(HC)
(Q(RQ))
(QR(RO)(RC)(RL)(RC))
(R(OR))
LR(C(QR))
LR(C(R(CR)))
LR(C(R(Q(R(C(RW))))))
LR(C(R(Q(R(LR)(CR)))))
LR(C(R(QR)))(CR)
LR(CR(QR)(LR)(CR))
LR(CR(QR)(RW))
LR(CR(QR))
LR(CR)
LR(CR)(QR)
LR(Q(R(C(R(LR)(CR)))))
LR(Q(R(CR)))
LR(Q(R(LR)(CR)))
LR(Q(R(QR)))
LR(QR(CR)(LR)(CR))
LR(QR(CR))
LR(QR(LR)(CR))
LR(QR)
LR(QR)(CR)
LR(QR)(QR)
LRQ(CR)
R(C(R(C(R(CR)))))
R(C(R(C(RO))))
R(C(R(C(RT))))
R(C(R(C(RW))))
R(C(R(CR(RT))))
R(C(R(CR)))
R(C(R(Q(R(C(RW))))))
R(C(R(Q(R(CR)))))
R(C(R(Q(R(LR)(CR)))))
R(C(R(Q(R(QR)))))
R(C(R(Q(RW))))
R(C(R(Q(RW))))(CR)
R(C(R(QR)))(CR)
R(C(RO))
R(C(RT))
R(C(RW))
R(CR(CR)(CR))
R(CR(CR))
R(CR(QR)(LR)(CR))
R(CR(QR)(QR))
R(CR(QR))
R(CR(QR))(CR)
R(CR)
R(CR)(CR)
R(CR)(CR)(CR)
R(CR)(CR)O
R(CR)(CR)T
R(CR)(CR)W
R(CR)(QR)(CR)

R(CR)O
R(CR)T
R(CR)W
R(CRQ(RW))
R(Q(R(C(R(C(RW))))))(CR)
R(Q(R(C(R(LR)(CR)))))
R(Q(R(CR)))
R(Q(R(Q(R(CR)))))
R(Q(R(Q(R(Q(R(CR)))))))
R(Q(R(Q(RW))))
R(Q(R(QR)(Q(RW))))
R(Q(R(QR)))
R(Q(RO))
R(Q(RW))
R(Q(RW))(CR)
R(Q(RW))(QR)
R(QR(CR)(CR))
R(QR(CR)(LR)(OR))
R(QR(CR)(OR))
R(QR(CR)(RW))(CR)
R(QR(LR)(LR))
R(QR(LR))
R(QR(OR))
R(QR(QR)(CR))
R(QR(QR)(OR))
R(QR(QR)(QR)(CR))
R(QR(QR))
R(QR)
R(QR)(QR)
R(QR)(QR)(CR)
R(QR)(R(OR))
RB
RG
RM
RN
RO
RP
RQ
RT
RU
RV
RX

Next topic: Printing User Manual

Printing User Manual

Printable Manual is provided in Adobe Portable Document Format (PDF). If Adobe Acrobat Reader is not installed in your computer, download from the Adobe Web site at http://www.adobe.com. Print this Manual by following the procedure given below:

1. Open **Windows Explorer**

2. Navigate to the folder **C:\Program Files\ZSimpwin\manual** by double-clicking each folder in the path until the **manual** folder is displayed.

3. Click the **manual** folder.

4. Double-click **Zsimp320**.

5. Click on the printer icon  in the tool bar to print the Manual.

The User Manual would be about 130 pages.

Next topic: File Structure and Management

File Structure and Management

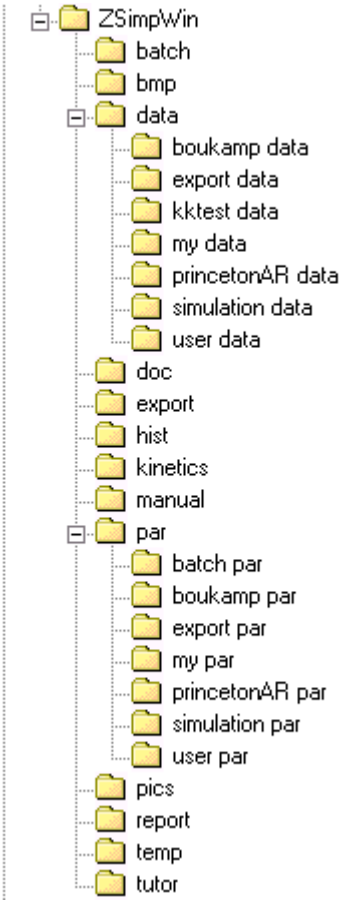
A brief description of the folders in ZSimpWin and file naming conventions.

Folders and subfolders
Files in ZSimpWin
File Naming Rules and Conventions
Saving various types of output

Next topic: Folders and subfolders

Folders and subfolders

The tree structure of the folders and subfolders created after installation is shown below:



Next topic: Files in ZSimpWin

Files in ZSimpWin

The names of installed folders and files are listed below:

Program files

Application	...	ZSimpWin.exe	
	...	Zsimp320.hlp	Essential files
	...	Readme.txt	Update information
		Cdclist.cdc	CDC list for User Library
		Zsimpopt.cfg	Run options

Sample run data

Impedance data	...\data\ ...\data\princetonAR data\ ...\data\boukamp data\ ...\data\user data\	*.txt, *dat, *dta, *z, *z60	Create a data folder and store impedance data
Parameter data	...\par\ ...\par\princetonAR par\ ...\par\boukamp par\ ...\par\ user par\	*.par	Create a folder matching with data folder before data analysis

Supporting files

History files	...\hist\	*.hst	Start and end times of iteration
Batch setup	...\batch\	*.cfg, *.mdl, *.lst, *.sta, *.tmp	Batch process setup files
Simulation data	...\data\simulation data\	*.sim	Saved in impedance data format
Simulation run results	...\par\simulation par\	*.par	Saved parameters
Picture files	...\bmp\	*.bmp	Pictures of listed models
Export data	...\data|\\export data\	*.dat	Reconstructed data
Temporary data	...\temp\	*.mat and *.*	Parameters at each iterations
Manual	...\manual\	Zsim320.pdf	Printable User Manual
Tutor	...\tutor\	*.pdf, *.doc, *.xls, *.bmp, *.txt	Tutorials and documents
Extrapolation test	...\data\kktest data\	*.txt	Testing extrapolation routine
Project Report	...\report\	*.prj, *.grp	Projects specified by a group of files
Plot files	...\pics\	*.emf, *.wmf, *.bmp, *.jpg	Saved plots
Documents	...\doc\	*.doc	Microsoft Word documents
Kinetics	...\kinetics\	*.dat	Reaction mechanism studies

File naming rules and conventions

The rules and conventions used in ZSimpWin are described below:

1. ZSimpWin is installed to the **C:\Program Files\ZsimpWin** as default. Another folder can be selected at the installation stage. This folder is the **Application Folder** and contains **ZSimpWin.exe**, **ZSimp320.hlp, ZSimpopt.cfg**, and **Readme.txt**. On registration, a registration key file (*.key) will be delivered from Princeton Applied Research. This registration file must be copied to this folder. Files in this folder are essential to run ZSimpWin. Sample data files and run results, technical notes, instructions, and program documentations are copied to its subfolders.

2. **Application folder** is abbreviated with **...** in this program and documentation.

3. A file is identified by folder name, file name, and its extension. The extension has less than or equal to three characters. ZsimpWin uses different extensions to facilitate data management.

4. Matching Data (Input) and Parameter (Output) folders are required. For example, **...\data\my data** and **...\par\my par**.

Impedance data are stored in the **..\data** folder or its subfolder. The subfolder must have the name**...\data\???? data** where "????" is an alphanumeric character string. Estimated parameters are stored in the **...\par** folder or its subfolder with the name **...\par\???? par\.** Impedance data and parameter folders with the same "????" are tied to each other.

The impedance data and the parameter folders are dynamically changed during program execution. The names of the current folders are saved when ZSimpWin is closed. At the next session, ZSimpWin starts with restoring the names of these folders.

Next topic: Saving various types of output

Saving various types of output

When EIS data analysis is completed in Iterate Mode, a dialog box **"Want to save with this filename?"** appears on the screen. Suggested file name is displayed as the dialog box title. Click on the **[Yes]** button. If you want to use a different name, you can click on the **[No]** button and then enter a name.

For pictures and documents, it may be desirable to save in your favorite folders. Click on the **[No]** button and save with the suggested filename in this folder or enter a filename in the **File name** edit box.

This routine has been extended to other functions. The suggested file names associated with various menus are assembled based on the rules given below:

Menu	**Destination folder**	**Default Name**
File | Open	DataPath	fname + ".txt" (or ".dat", ".dta", ".z", ".z60", etc.)
File | Retrieve Parameters	ParPath	fname + ", " + CDC + ".par"
File | Save Parameters	ParPath	fname + ", " + CDC + ".par" (Iterate Mode)
	...\par\simulation par\	CDC + ".par" (Simulate Mode)
	...\hist\	fname + ", " + CDC + ".hst"
	...\temp\	fname + ", " + CDC + ".mat"
File | Save Simulation Data	...\data\simulation data\	CDC + ".sim"
File | Save Impedance Data	DataPath	fname + ".dat"
Output | Save Plot (1 data set) Multiple in a project group	...\pics\	fname + ", " + CDC + plot style + ".emf" (or "..wmf", ".bmp", ".jpg) groupname + ", " + plot style + ".emf" (or ".wmf", ".bmp", ".jpg")
Output | MS Document	...\docs\	fname + ", " + CDC + plot style + ".doc"

... :	Application folder. Default = C:\ZSimpWin\.
Fname :	Filename without folder name and file name extension (e.g., "ASTM dummy cell").
CDC :	Circuit Description Code.
DataPath :	Impedance Data Input folder (...\data\, ...\data\princetonAR data\, ...\data\my data\, etc.)
ParPath :	Parameter Output folder (...\par\, ...\par\princetonAR par\, ...\par\my par\, etc.)
Plot style :	Current plot style ("N", "B", "R", "A", "C", or "E")

Dialog Screens

Description of the functions associated with the buttons in dialog screens.

Input/Output

- Open File
- Paste Z Data
- Save Parameters
- Retrieve Parameters

Standard operations

- Select Model and Run Mode
- Edit Parameters and Run
- View, Print, and Copy Results
- Options

Batch processing

- Batch Process Setup and Run
- Check Progress
- Popup Menu

Document

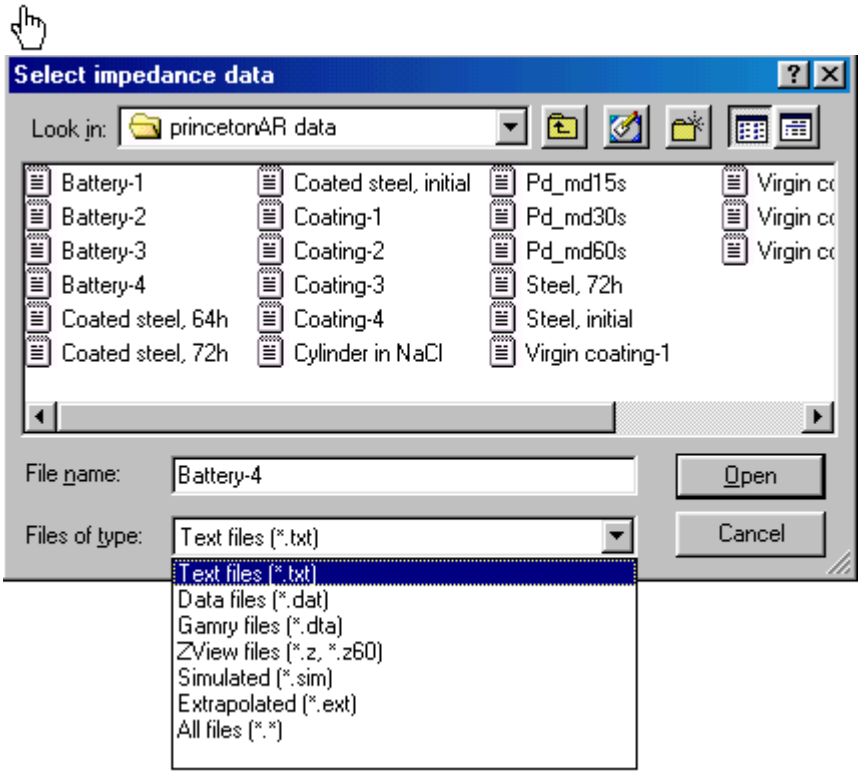
- Select Print Items
- Print Project Group

Extrapolating data

- Extrapolate using Kramers-Kronig Relations

Open File

This will display a standard file-open dialog; choose the drive and folder, and select a file for analysis. Supported file types are text files (*.txt, *.dat), Solartron's ZView formats (*.z60, *.z), and Gamry's data format (*.dta).



Next topic: Paste Z Data

Look in
Displays the current folder. Navigate to the desired folder by double-clicking each folder in the path until this folder is displayed.

Files of type
Selects a file type. Only the files of the selected type will be listed.

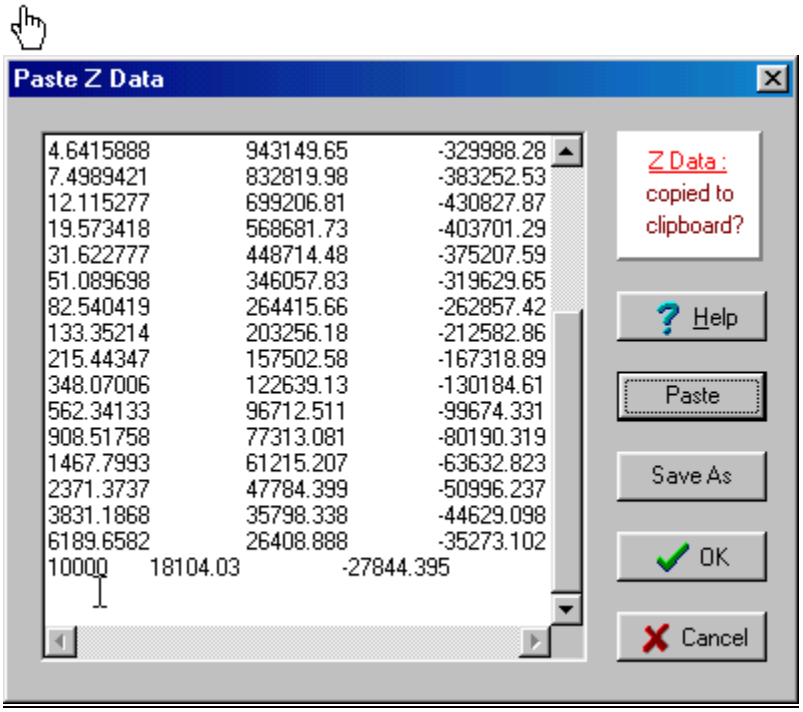
Files in selected folder
Displays the files in the selected folder of the selected type.

Open button
Click this button to open the selected file.

Paste Z Data

Paste Z Data from Windows clipboard. All the data points should have been copied to Windows clipboard. Each data point should be represented by frequency, real component of impedance, and imaginary component of impedance.

This menu has been initially designed to import an impedance data set from PowerSine Database using the "**Edit | Copy Z Data"** function in the PowerSine (See Application Example 8: Pasting Z Data from PowerSine). It would work with any other applications capable of copying the data points to the Windows clipboard.



See Application Example 8.

Copied to Clipboard?

Impedance data must have been copied to the Windows clipboard as a text file from other application such as PowerSine.

Paste Data

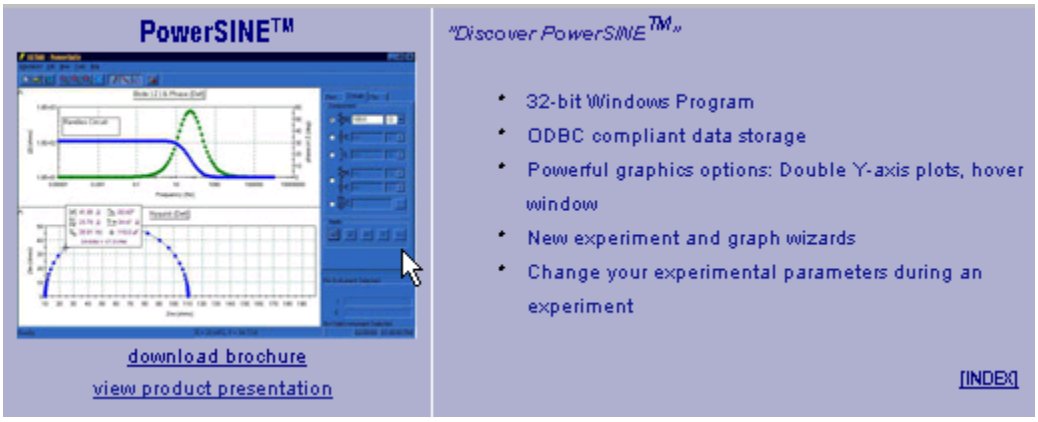
Pastes the data to the memo area. These data arbitrarily named as "**unknown.txt**" are used for analysis.

SaveAs

Saves the current data ("unknown.txt") with a different name.

About PowerSine

PowerSine is a powerful data acquisition software developed by Princeton Applied Research. Electrochemical Impedance Spectroscopy data are stored in Microsoft Access database format. This format provides flexibility in data export. These data can be exported to Excel format, text format, or copied to Windows clipboard.

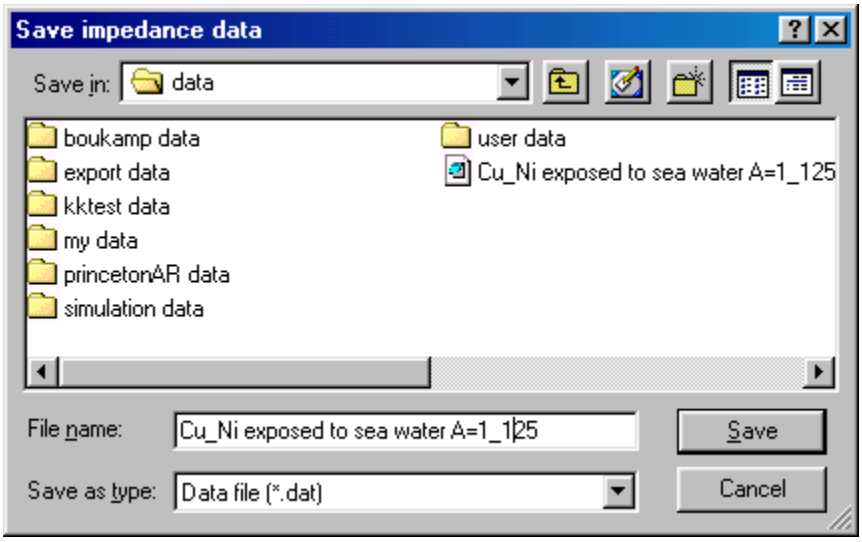


Visit the Princeton Applied Research site at http://www.princetonappliedresearch.com

and download the brochure to discover the power in the **PowerSine**.

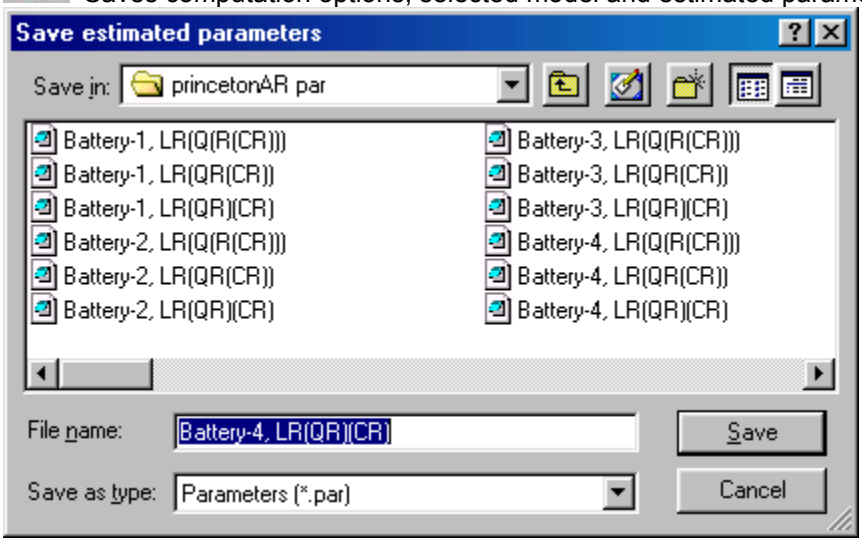
Save impedance data

Saves the current impedance data as a text file. Simulation run results, data accessed from **Solartron** or **Gamry** data formats can be saved as a text file.



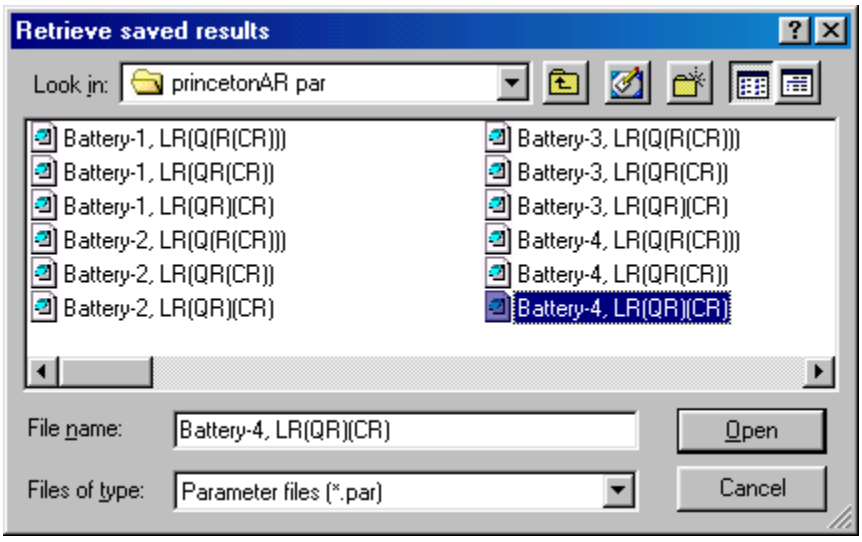
Save Parameters


Saves computation options, selected model and estimated parameters.



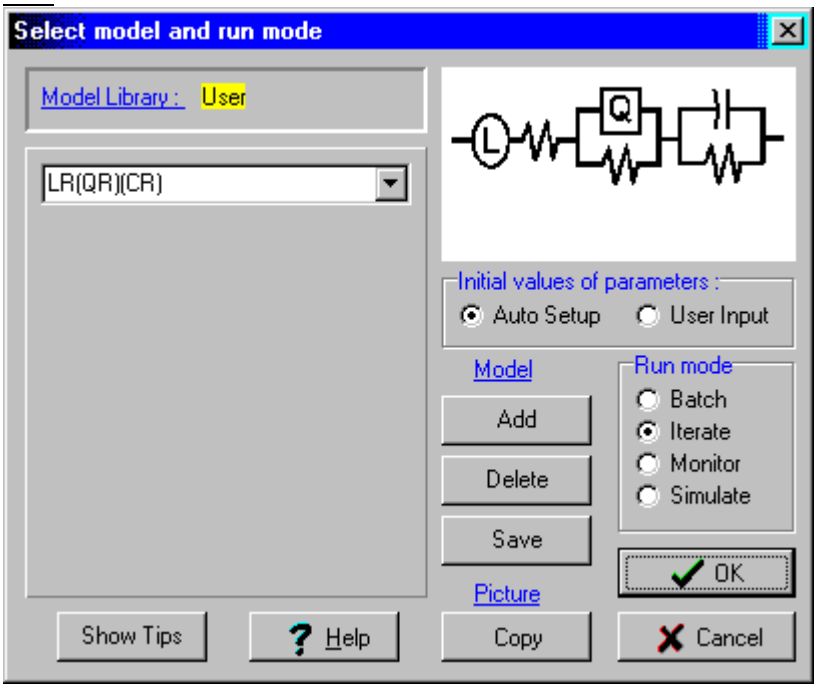
Retrieve Parameters

 Retrieves analysis results from a file containing the weighting factor, model, estimated parameters, and uncertainties of these parameters.



Select model and run mode

 is used to select a model and start computation.



Model Libraries
There are two libraries: System Library and User Library. The System Library consists of 75 Circuit Description Codes associated with models. These codes cannot be modified or destroyed. It is recommended to copying the System Library to the User Library and to customize by adding or deleting codes.

Drop-down list area
The area list of Circuit Description Codes are displayed with a mouse button click on the down arrow.

Model Add
Enter CDC code in the edit box and add to the list. The validity of the code is checked before addition.

Model Delete
Deletes the selected code from the list.

Model Save
Save updated list to a file. This list is loaded at program startup.

Model Copy
Copy the picture to Windows clipboard.

Model Selected model
Shows selected model.

Model Initial Parameters
Initial parameter are setup automatically (Auto Setup) by ZSimpWin by default. In special occasions, these parameters may have to be entered (User Input). Computation starts with these parameters.

Run modes

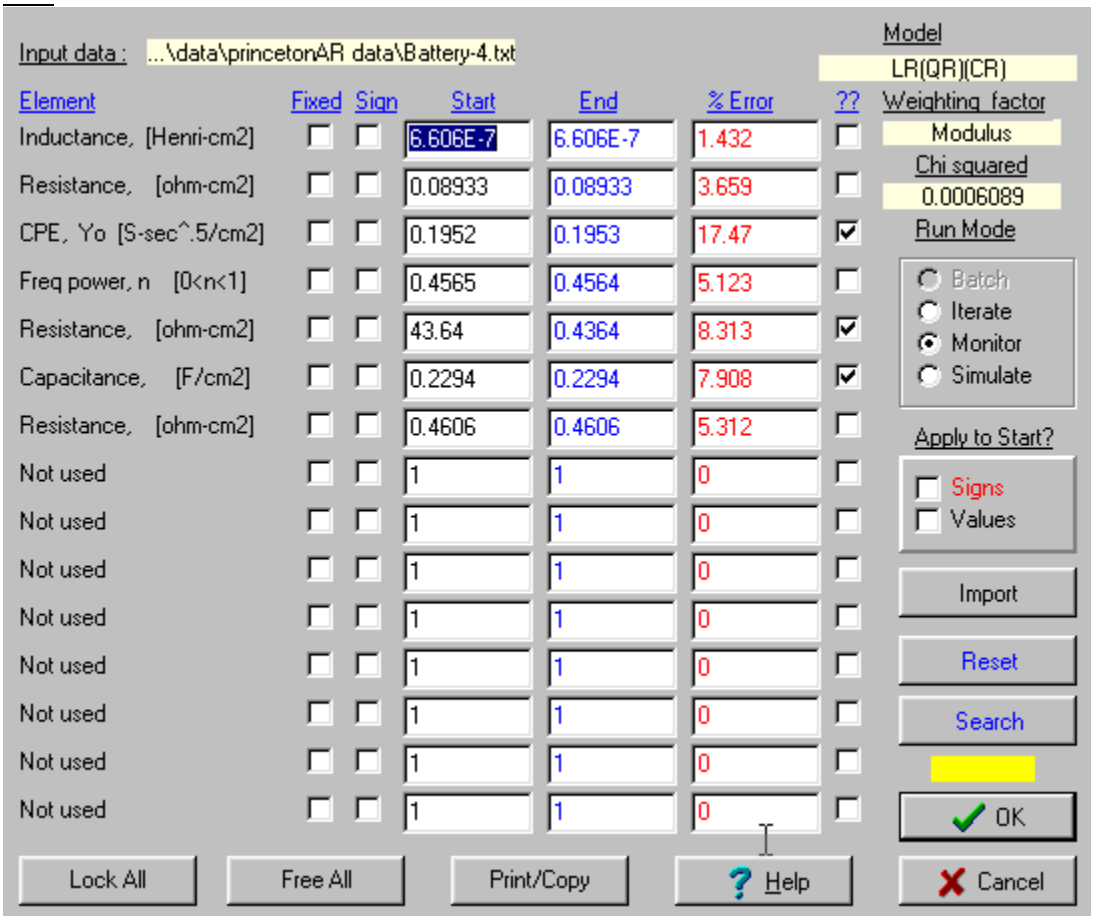
- **Batch**: Multiple files are processed in sequence using several models. Results are saved in separate files.
- **Iterate**: Analyzes and displays final results for a file and a selected model.
- **Monitor**: Pause after one iteration. Can adjust several parameters before the next iteration.
- **Simulate:** No optimization. Compute with parameters associated with a model.

Model OK
Accepts selected model and starts computation when Auto Setup was selected. Leaves this dialog screen.

Model Cancel
Leaves this dialog without changing anything.

Edit Parameters & Run

This dialog screen shows the data file name, selected model, weighting factor, initial parameters, final results, uncertainties of estimated parameters, and χ^2 (chi squared). When the OK button is clicked after editing parameters, this dialog box is closed, and then computation starts when necessary. This dialog is not applicable to batch processing mode.



Next topic: View, Print & Copy Results

Fixed or variable

Any parameters can be taken as constants during optimization. In a simulation run, all the parameters are taken as constants.

Sign of parameters

Signs of parameters. Checked parameter is negative.

Start values
The start values used for computation in the most recent iteration. At the beginning of data analysis (i.e., the 0th iteration), these values are automatically set to an initial guess with the **Auto Setup** option or to the values provided by the user with the **User Input** option.

End values
The results obtained after the most recent iteration using the start values. These results are associated with a local minimum. The end values for the last iteration represent the final results, i.e., the absolute minimum of the chi-squared.

Run mode selected
Selected run mode is displayed. Run modes are batch, iteration, monitor, and simulation. Do not change the modes.

Simulation mode
Requested simulation mode?

Apply to Start
This is associated with the **User Input** option. The user can change the sign and/or values of the initial guess provided with the **Auto Setup** option. Changes are applied to sign and/or values. Computation starts with the updated initial guess.

Import
This feature is associated with the **User Input** option for the srat values of the parameters. Instead of typing their values, imports the final results for other data obtained using the same model.

Parameter labels
Identification of parameters.

OK
Updates changes in parameters and returns to the main window and starts computation if requested. ZSimpWin checks various conditions to identify the type of the request and takes necessary operations (no action, compute in iteration mode, monitor mode, or simulation mode).

Cancel
Cancels the function and closes the window. Changes in data fields are discarded.

File name
Displays the name of the selected file including its file path.

Model
Selected model.

Chi-squared
Displays the minimum of the $\chi 2$ value, i.e., the goodness of fit to the selected model.

Chart title
Displays the file name, weighting factor, and selected model.

Search
Resets and waits for the next iteration. Computation will start when the **OK** button is clicked. Pause after one iteration is implicitly requested by the user.

Reset
Replaces the initial parameters with final results. This function has been intended to be used with manual edit of several parameters. A combination of **Reset** and manual edit is similar to **Search**. The start values for the next iteration are input by the user with the Reset and manual edit, whereas they are determined by ZSimpWin with **Search.** Optimization is performed at the next step. In both cases, pause is implicitly requested by the user.

Print/Copy
Opens a dialog screen providing options to print results in several different formats and to copy these results to Windows clipboard.

Free All
Sets all the parameters as variables. All the values are changed during optimization.

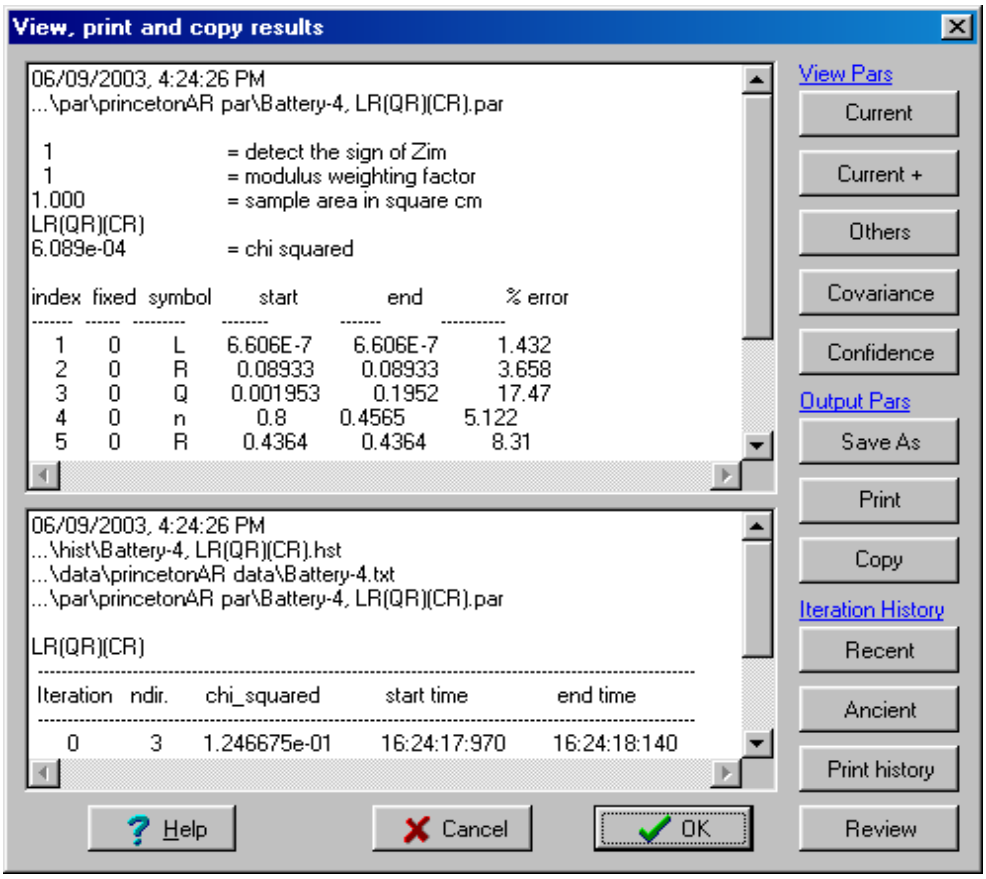
Lock All
Set all the parameters as constants.

View, Uncertainties of parameters
Std. error or % error. The % error = 100 * (std. error) / (estimated value).

Directions considered
A check mark in the "??" column represents a direction. Several parameters are most likely to have the most significant effect on reducing $\chi 2$. Only the directions associated with these parameters are tested to find the start point for the next iteration.

View, Print & Copy Results

 to view analysis results, iteration history, and details of computation steps. These results can be printed or copied to Windows clipboard.



Because ZsimpWin already knows that computation has been performed, the parameters and iteration history for current data are displayed on the opening of this dialog.

The memo area at the top is to display estimated parameters.

Current to view the results for the current data.

Current + to append the iteration history to the parameter file.

Others to view the results for other data.

Covariance to view covariance matrix

Confidence to confidence regions for two selected parameter.

SaveAs to save the displayed contents.

Print	to print the contents in the viewing area. These contents can be parameters only or (parameters + history).
Copy	to copy the contents to Windows clipboard.

The rectangle at the bottom is to display iteration history.

Recent	To display the iteration history for the current data.
Ancient:	To check the history created for other data.
Print history	To print the history file.
Review	To see the variation of parameters with iterations (See Review Iteration Steps).

Print View current
Load the parameters estimated for the current data to the Memo.

Print View current +
Appends the history at the end of the parameter file.

Print, SaveAs
Saves the content in the memo area as a file.

Print, Recent
The iteration history for the current data.

Print View others
Read other parameter files and display in the Memo.

Print Ancient
Views the iteration history for other data files.

Print, Print history
Prints the iteration history displayed in the memo area.

Print Copy to clipboard
Copy the contents in the Memo to the Windows clipboard.

Print, Parameter display area
The memo area to display estimated parameters.

Print, History display area
The memo area to display a history file.

Print Print
Print the contents in the Memo.

Review Iteration Steps

The changes of the parameters and the chi-squared are also automatically saved as a file. These results can be displayed as parameters vs. iteration number or chi-squared vs. iteration number plots.

A. When does iteration stop?

Iteration is terminated when the global minimum of the chi-squared is reached. The chi-squared obtained after an iteration is associated with a local minimum. Iteration proceeds by moving from one local minimum to another towards a lower value. When the global minimum is reached, there is no place to move, because a lower minimum is not available.

Version 2.00

Condition 1:
(a) none of the parameters is changed appreciably (less 1%), and
(b) the chi-squared value is practically not changed (less than 1e-5).

Condition 2:
Iteration counter reaches the maximum set value (default = 10).

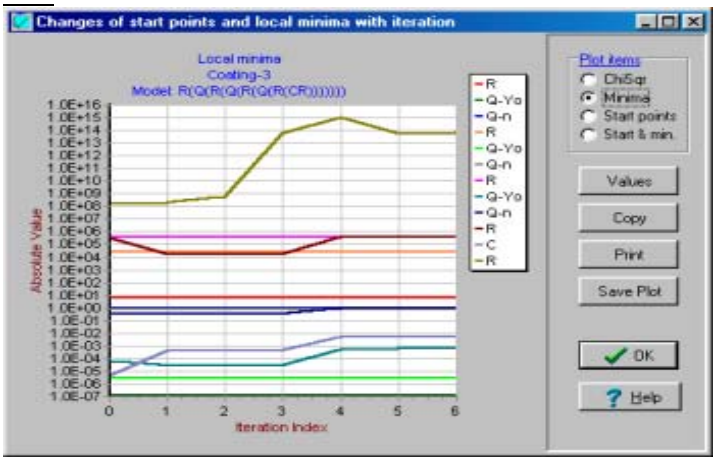
Versions higher than 2.00

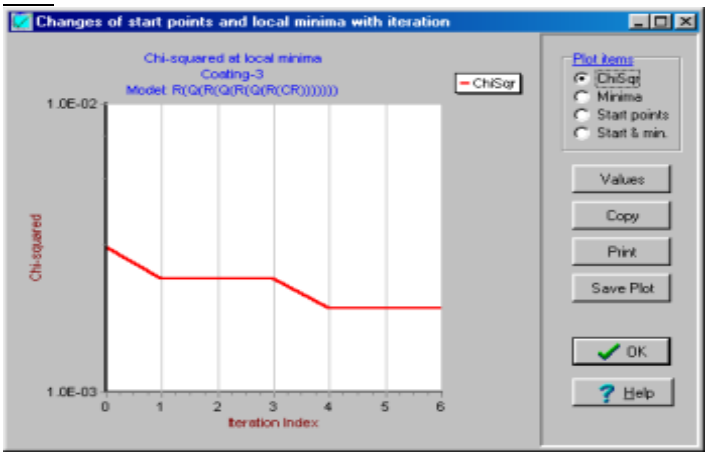
Eliminated unnecessary iterations by modifying the Condition 1.

After the 1st, 2nd, and 3rd iterations: (a) and (b).
After the 4th, 5th, ... 10th iterations: (b).

A parameter with very high uncertainties is changed significantly without affecting the chi-squared value. Even though the desired solution has been obtained, iteration is expected to continue until the maximum set value is reached.

At initial stage, we have to be conservative because we started with a rough initial guess. More stringent criteria were employed to prevent premature termination. At later stage, only the chi-squared value was evaluated to avoid unnecessary iterations. Tests have been performed with 30 sample data applying various models. About 70 % of these cases achieved the reductions ranging from 15 to 70 %, and others no reduction. Average reduction of computation time was about 30 percent. This modification did not cause any loss of computational accuracy.





Review, Select plot
Select the plot to display. Parameters vs. Iteration Number or Chi-squared vs. Iteration Number.

Review, Values
Examine how the values of the parameters and chi-squared changed with iteration.

Review, Copy
Copy the plot to Windows clipboard.

Review, Print
Print the plot and the variation of the parameters and the chi-squared in Landscape mode.

Review, Save Plot
Save the current plot as a file to the ...\pics\ folder. Graphics format is selected by setting the plot format in the Options dialog box. Available formats are Enhanced Metafile (EMF), Windows Metafile (WMF), Bitmap (BMP), and JPEG(JPG).

Review, OK button
Close the screen.

B. What can we learn from these plots?

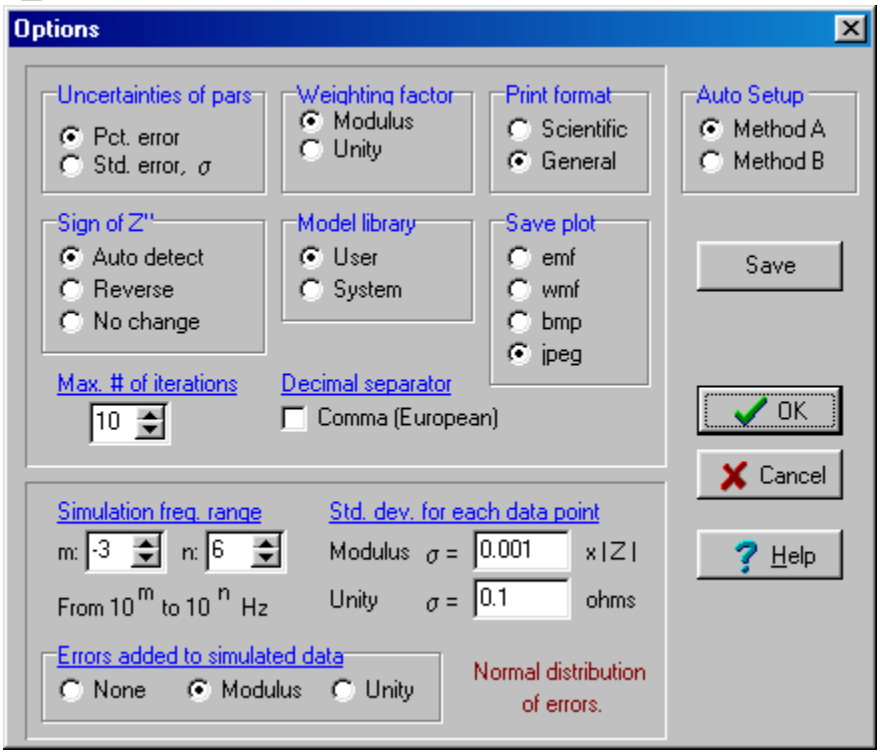
When the **[Print]** button is clicked, the plot, the variations of the parameters (See Change of parameters with iteration) and the chi-squared (See Change of chi-squared with iteration) are also printed on a single page. We could get the following information:

- Twelve parameters are associated with the selected model.
- High uncertainties are involved in the last parameter (1e+14 ohms).
- The local minima of the chi-squared associated with iterations: the 1st, 2nd, and 3rd are slightly different. the 4th and the 5th are very close. No change from the 5th to the 6th. The small differences are detected by examination of the tables.
- Six local minima were searched.
- Iteration was stopped when the chi-squared did not change.
- The local minimum reached after the last iteration is equal to the global minimum of the chi-squared. The parameters associated with this minimum is the optimum solution.

Next step: Batch Process Setup and Run

Run Options

Changes the specifications associated with computation.



Uncertainties of parameters

"**Std. error**" or "**% error**" (**default is % error**). Uncertainties of estimated parameters are expressed in standard errors. Estimated parameters may be expressed in the statistical expression, a ± da, where da is the standard uncertainties in the estimate of the parameter. For practical purpose it is more convenient to express in % error. This error is defined by

% Error = 100 * (std. error) /(estimated value).

Large uncertainties are associated with insignificant effect of the parameters on the calculated curve. Even though an excellent fit is obtained, determined parameters may not be meaningful. It is also possible that its effect is combined with dominant effects of other parameters.

Sign of Zimag

Because imaginary components of data points are generally negative, impedance data are actually analyzed with -Z" rather than Z". Data acquisition systems might save imaginary components either in Z" or –Z" (i.e., after reversing the sign). With the **Auto Detect** option selected, ZSimpWin checks the signs of the imaginary components and reverses the sign if necessary.

With the **Auto Detect** option, it has been assumed that more than half of the data points lie on the first and second quadrants. If this assumption is not valid, uncheck the **Auto Detect** and check the **reverse sign** or **do not change** whichever is adequate.

Auto Detect
Automatically detects the sign (**Default = checked**):

Reverse sign
Change the sign of Zimag.

No change
Do not change the sign of Zimag.

Weighting factor
To determine optimum parameters, the least squares fit principle is applied, i.e., minimization of the sum of the residual squares. Normal distribution of standard deviations for each data point is assumed. The standard deviations are assumed to follow a certain behavior. Available weighting factors are as follows:

Factor	weight (re)	weight (im)	Assumption on standard deviations
Unity	1	1	Std. dev is constant.
Modulus	|Z|	|Z|	Std. dev. is proportional to |Z|.

Change this factor by clicking the button (**Default = Modulus**).

Model Library
Two lists with different characteristics are provided for selection.

(a) System Library: consists of 75 codes associated with model. Cannot be modified or destroyed.

(b) User Library : Can be changed by the user.

Create the User Library by copying the System Library and then customize by adding or deleting codes.

Print format
Final results can be printed in scientific or general (fixed or scientific depending on the value of a parameter) format. **Scientific format** provides better data alignment because the same number of data fields is used to print floating values. **General format** provides convenience in reading, however, alignment is poor because the number of data fields to print a floating value depends on the magnitude of the value. One of these options can be selected by the user.

Save plot format
Select the format to save the displayed plot in Enhanced Metafile (*.emf), Windows Metafile (*.wmf), Bitmap (*.bmp), or JPEG (*.jpg). This file can be inserted to a document. **Default = Enhanced Metafile**.

Simulation frequency range
Sets the frequency range for a simulation run.

Decimal separator
Europeans prefer using commas as decimal separators. Check the radio button "**Comma(European)**" to select this format. Selection of this option requests writing results using commas instead of periods for

floating numbers (e.g., 1,24e-09 and 23,457). Dialog screens also display the numbers using this format.

Max # of iterations
A criterion to stop computations. Allowed range is **5-20**.

Standard deviation for each data point
The standard deviation for each data point is assumed to be independent. With unity weighting, the standard deviation is assumed to be constant for all data points. With modulus weighting, it is assumed to be a constant fraction of the absolute value of the impedance.

Errors added to simulated data
Errors can be added to simulated data points. Based on the standard deviation for each data point, the error to be added is estimated using a random number generation routine.

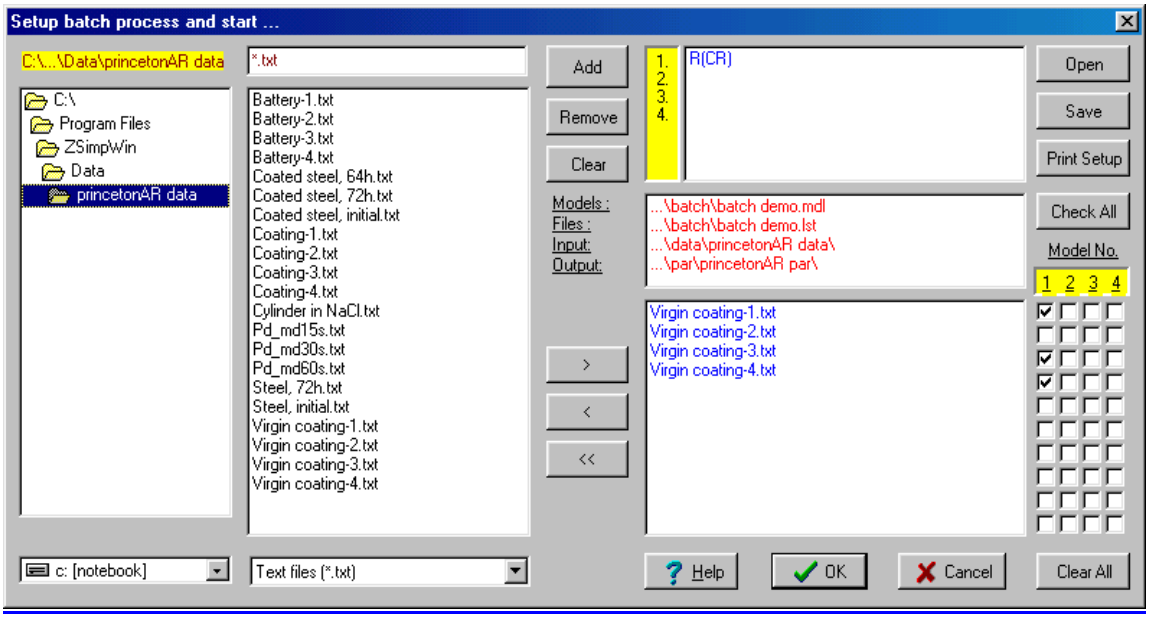
Auto Setup
Select Method A or B before running in Iterate Mode or Batch Processing Mode. When desired results are not obtained with Method A (default), try Method B. This option is not saved unlike other options. Run **batch demo with z, Auto Setup B** after selecting the **Method B**.

Save options
Saves the selected options to **zsimpopt.cfg**. These options are read at program startup.

OK button
Changes the options and leaves the dialog screen.

Batch processing mode setup

Analyzes multiple files in sequence using a model.



See Flowchart: batch process setup.

Open batch setup
Loads the list of files saved as a batch name.

Save batch setup
Save the list of files as a batch name.

Print batch setup
Prints batch setup

Add model to list
Adds a model to the model list.

Remove model from list
Removes a model from the model list.

Clear model list
Removes all the models in the list.

Right button
includes a selected file to the list.

Left Button
removes a file from the list.

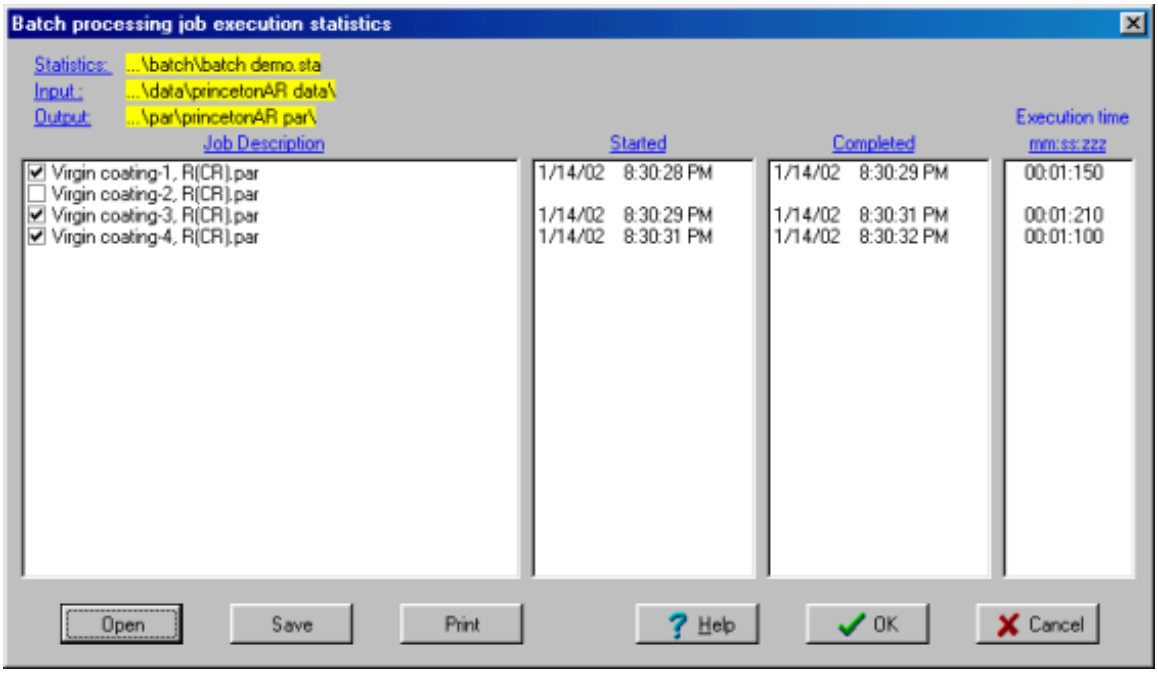
Clear button
clears the file list.

Display selected jobs
Check marks indicate selected jobs.

Exclude all jobs
Excludes all jobs in the job list.

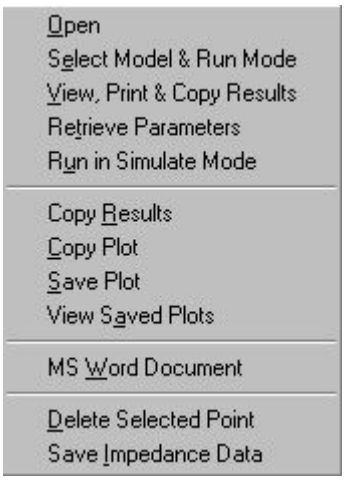
Check progress

Start and end times of each job are saved and displayed on the screen. Execution time is also displayed in minutes, seconds, and hundredths of a second. If the batch process has not been completed, the current status is displayed.



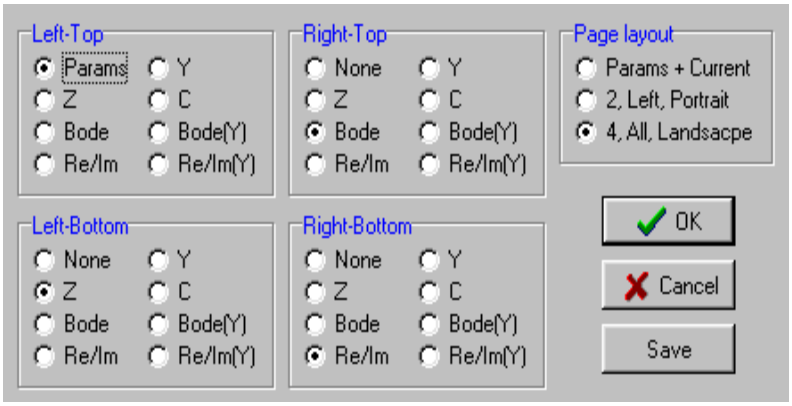
Popup Menu

Click the right mouse button to access the popup menu. Most of the menu items in the main menu can be selected.



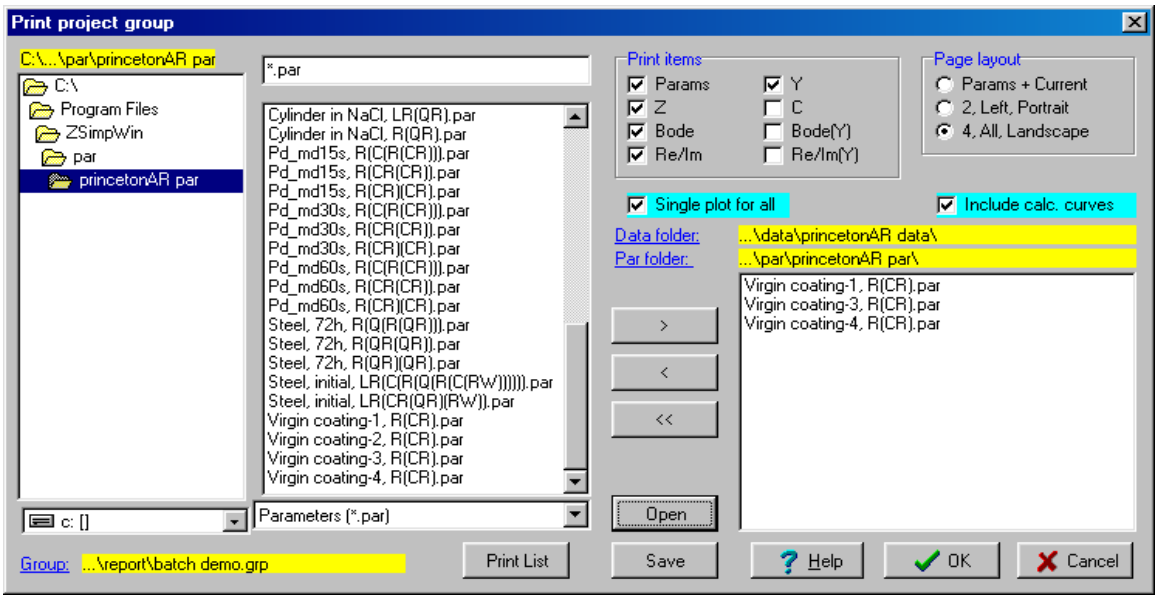
Print Item Selection

 Prints different items on a page.



Print Project Group

EIS analysis results can be printed at a time. A project group is a list of the parameter files. This group can be saved as a file and accessed in a later session.



Next topic: Report Preparation

Report, Right button
Includes a selected parameter file to the list

Report, Left button
Removes a parameter file from the list

Report, Clear button
Clears the files in the list

Report, Open
Opens a group and displays the list of the files in the group.

Report, Save
Saves the list of the files as a group.

Report, Print List
Prints the list of the files in the selected group.

Drive id
Selected drive id.

File filters
Allowed file filters.

Selected filter
Displays the selected filter.

Files in selected folder
Displays the files of select type in the selected folder.

Directory List
Directory structure to select a folder.

Plot style
Plot styles.

Bode, Absolute
The vertical axis on the left (absolute value of Z or C) can be linear or logarithm.

Print items
Selects the items to print on a page.

Selected files
The names of the files selected.

Report, OK button
Leaves this dialog box and prints the plots for the members in the selected group. If the **single plot for all** is checked, leaves this dialog and displays the requested plot. Click on the **[Printer]** button in the tool bar to print the current plot.

Files in a group
The files in the selected group.

Group name
The name of the project group containing selected parameter files.

Directory label
Displays the name of the selected folder.

Single plot for all
When this checkbox is checked, all the data sets are plotted together. One plot is generated.

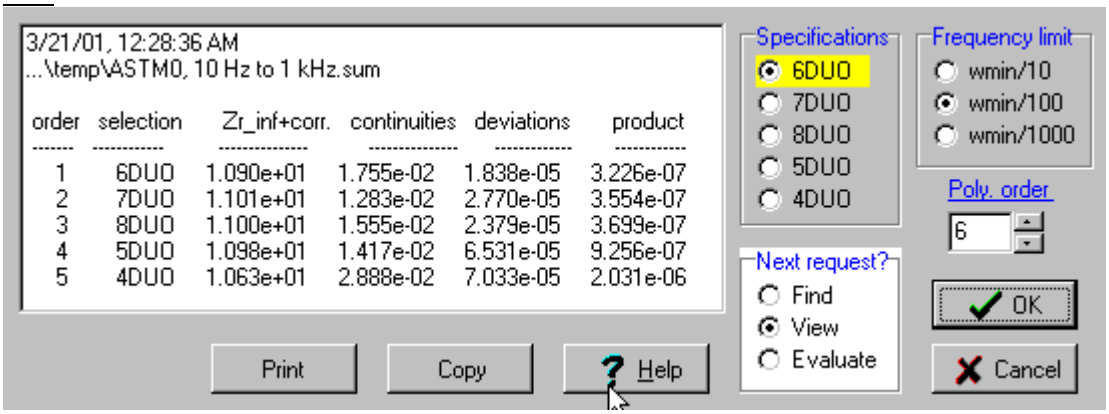
Include calc. curves
A plot can contain only measured data points for the members in a group or include calculated curves.

Data folder
The name of the data folder.

Parameter folder
The folder parameter files were selected. All the files should be present in the same folder.

Kramers-Kronig relations

Click on the **Apply Kramers-Kronig** in the **Extrapolate** menu to extrapolate data to a low frequency.



Determine extrapolations by approximating the real and imaginary components of the impedance with polynomials (See reference), inserting into the Kramers-Kronig relations, constructing linear equations, and then solving these equations for the polynomial coefficients.

$$Z''(\omega_i) = -\frac{2\omega_i}{\pi}\int_0^\infty \frac{[Z'(x) - Z'(\omega_i)]}{(x^2 - \omega_i^2)}\,dx$$

$$Z'(\omega_i) = Z'_\infty + \frac{2}{\pi}\int_0^\infty \frac{[xZ''(x) - \omega_i Z''(\omega_i)]}{(x^2 - \omega_i^2)}\,dx$$

Extrapolations depend on the order of the polynomials. Click **Find** to find the results for the polynomials of different orders (4 to 8). Click on the **[OK]** button.

Select an order of the polynomials, and click **View** to examine corresponding extrapolated segment. Click **Evaluate** to compute the impedance using the extrapolated data.

Print: Prints the results and displayed plot (See Print Extrapolation Results).

Copy: Copies the results to Windows clipboard.

Reference:

J.M. Esteban and M.E. Orazem: "On the Application of the Kramers-Kronig Relations to Evaluate the Consistency of Electrochemical Impedance Data," J. Electrochem. Soc., Vol. 138, No. 1, 1991, pp. 67-76.

Next request?
Can request a service (a) Find, (b) View, and (c) Evaluate after setting the options. They are expected to be executed in sequence. Select one of these services and click on the **[OK]** button.

Specifications
A character string specifying the order of the polynomial, preferred condition, and the number of decades extrapolated below the lowest measured frequency.

Order of polynomials
The order of the polynomials (4 to 8) for extrapolations. The number displayed in this box is used for computation.

Print, extrapolate
Print the contents and the displayed plot.

Copy, extrapolate
Copy the contents to Windows clipboard.

OK button
Services the selected request.

Frequency limit
Extrapolate by one decade or two decades below the lowest measured frequency (wmin).

Extrapolation results
Displays the value of the Z'(inf) + corrections, continuities, deviations and their product for each order of the polynomials.

Report Preparation

Instruction to use the advanced features for efficient report generation.

- Printing Results for Multiple Data Sets
- Import/Export Functions
- Single-page Document
- Working with a Word Processor

Next topic: Printing Results for Multiple Data Sets

Printing Results for Multiple Data Sets

Results for multiple data sets can be printed at a time.

A. Selecting files to print

1. Click on the 

2. Create a group by adding the parameter files to print
3. Save the group as a file.
4. Select one of the combinations of the items to print.
5. Click on the **[OK]** button

B. Accessing saved group

This is equivalent to retrieving the analysis results for a group of data sets.

1. Click on the 

2. Click on the **[Open]** button and select a saved group.
3. Select one of the combinations of the items to print.
4. Click on the **[OK]** button.

C. Batch processing run

A group is also created after a batch processing run. Print this group by following the same procedure given in **B. Accessing saved group**.

Next topic: Import/Export Functions

Import/Export Functions

Prepare a report by retrieving the analysis results, exporting data, and then importing to a document..

A. Exporting Data
Data can be exported by copying the results to Windows clipboard, copying displayed plot to Windows clipboard or saving the plot using the following buttons:

It is recommended to use the default size Window. Do not maximize. You can use large fonts for the chart title, axis labels, and legends. Before exporting data, select large fonts by checking the **Large fonts** in the tool bar.

A plot can be saved in Enhanced Metafile (emf), Windows Metafile (wmf), Bitmap (bmp), or JPEG(jpg) format. Default format is Enhanced Metafile. Choose the format by clicking on the  button and checking the radio button associated with the file format.

B. Importing Data
A document can be prepared in electronic form by pasting analysis results and plots. For sophisticated formatting of the document, use your word processing application (See Working with a word processor).

B.1. Pasting text from Windows clipboard

1. Copy results 
2. **[MS Word document]** 
3. **[New]** to create a new document.
4. Paste to a document

B.2. Pasting plot from Windows clipboard

1. Copy plot 
2. **[MS Word document]** 
3. **[New]** to create a new document.
4. Paste to a document

B.3. Inserting plot from file

1. Save plot as a file  (ZSimpWin)
2. Insert to a document (**Insert | Picture | From File** in Microsoft Word)

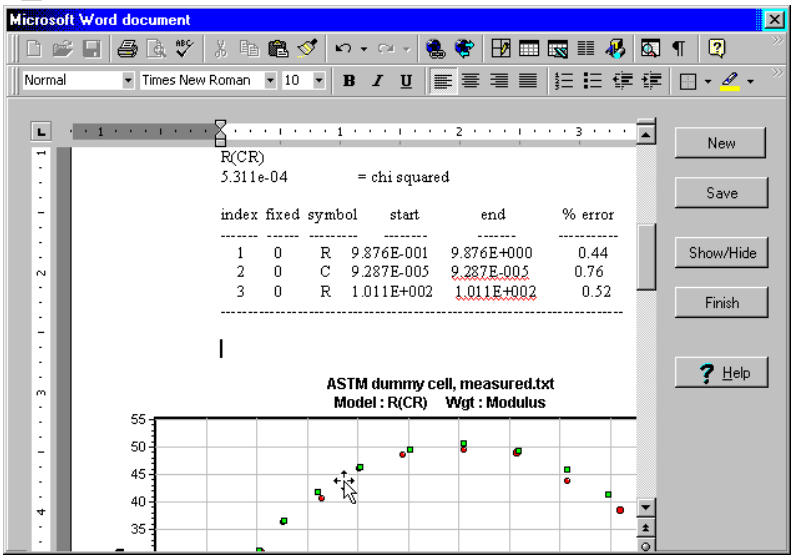
Next topic: Single-page Document

Single-page Document

Prepares a Microsoft Word document by pasting analysis results and a plot.

[Copy Plot] → [MS Word Document] → Paste → [Copy Results] → [MS Word Document] → Paste → Save document

When the **[Save]** button is clicked, a save filename is suggested. This name consists of input filename, selected model name, and the style of the displayed plot. Click on the **[Yes]** button to accept this name. This file is saved to the **...\doc** folder. If you click on the **[No]** button, you are requested to enter its name and its destination.



Toolbars
Toolbars of Microsoft Word.

New document
Create a new document

Save document
Save the current document with the suggested name or a user-supplied name.

Finish
Close the document.

Show/Hide
Show or hide the toolbars. Paste is allowed only when the toolbars are visible.

Help, MS Word document
A brief instruction on preparing a single-page document.

Working with a Word Processor

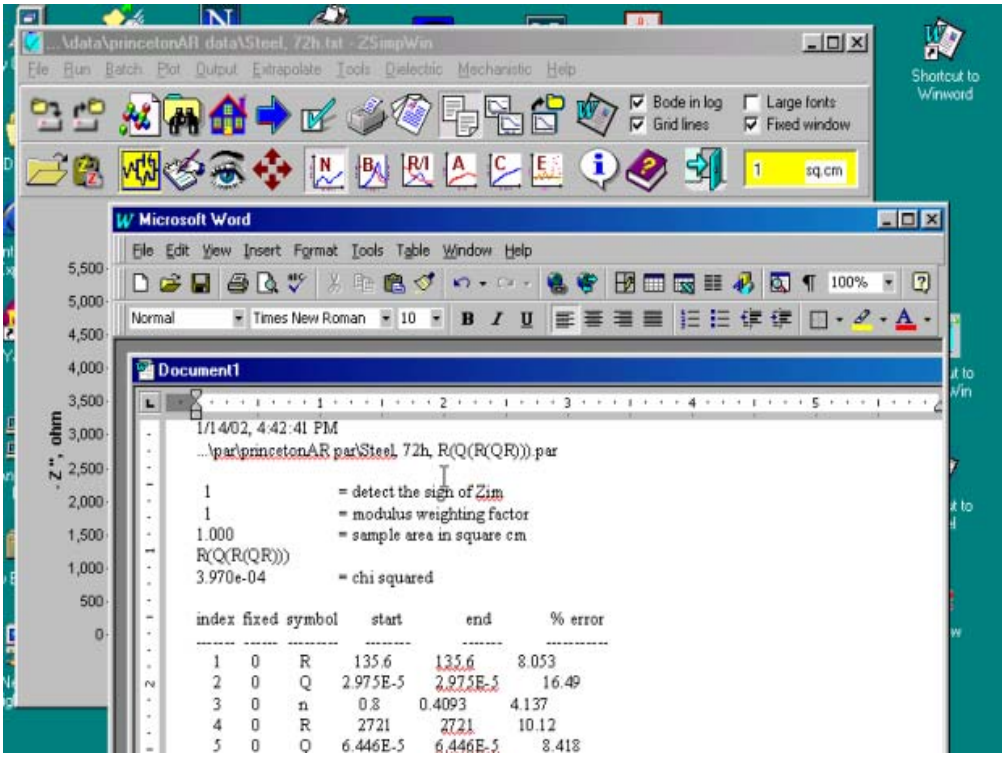
For sophisticated formatting of a document, use a word processor instead of the **[MS Word document]** in the toolbar.

1. [Copy Plot] → Open MS Word → Paste → [Copy Results] → Paste → Save document → Print

2. [Save Plot] with emf format → Open MS Word → Insert to document → [Copy Results] → Paste → Save document → Print

3. [Save Plot] with bmp format → Open Paint → Edit picture → Open MS Word → Insert to document → [Copy Results] → Paste → Save document → Print

It would be convenient to place its shortcut at the top-right corner of the Desktop.



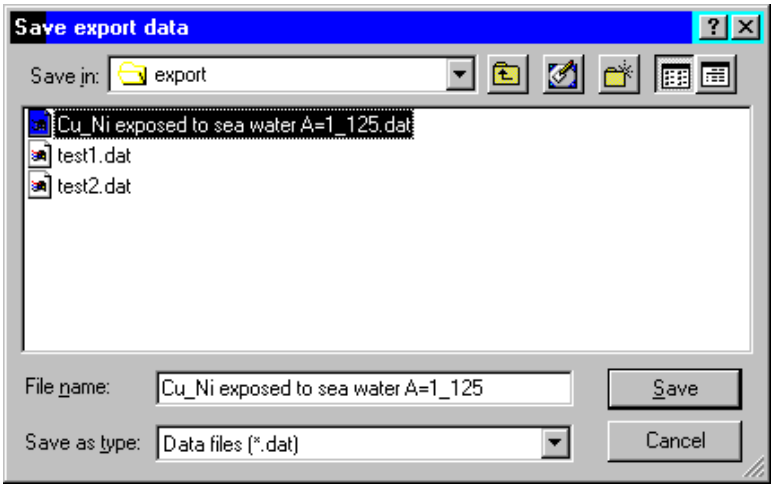
Tools

Special purpose tools.

- Export Data
- Enter Sample Area
- Create New Folder
- Append Header Lines
- Change Chart Titles
- Edit Sample IDs
- Edit Simulation Parameters
- Reading the Coordinate of a Data Point
- Deleting Data Points
- Close Examination of a local area
- Get Pseudocapacitance
- Specify Image Viewer

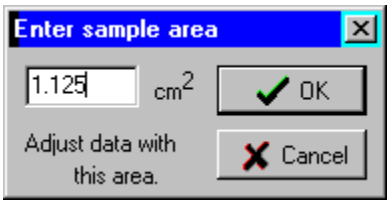
Export Data

Data can be exported to various formats. Available formats are "Impedance", "Bode", "Real / Imag", "Admittance", and "Capacitance". If data analysis were completed, the results would be also exported. Data are exported to the **.../export/** folder with ***.dat** as file extension.



Enter Sample Area

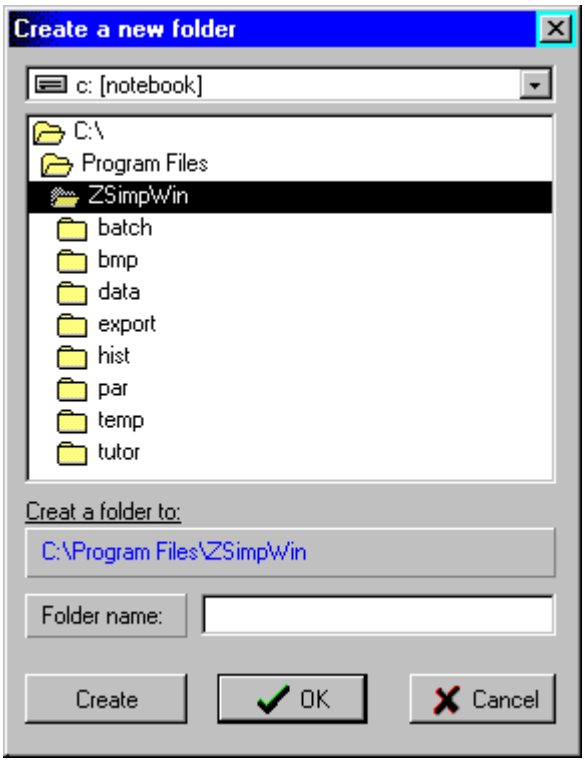
Sample area in square centimeters. Default is 1.0 square centimeter. This area should be specified immediately after opening a file. If this area is equal to 1.0 square centimeter, area unit is not attached to axes labels.



Next topic: Create New Folder

Create New Folder

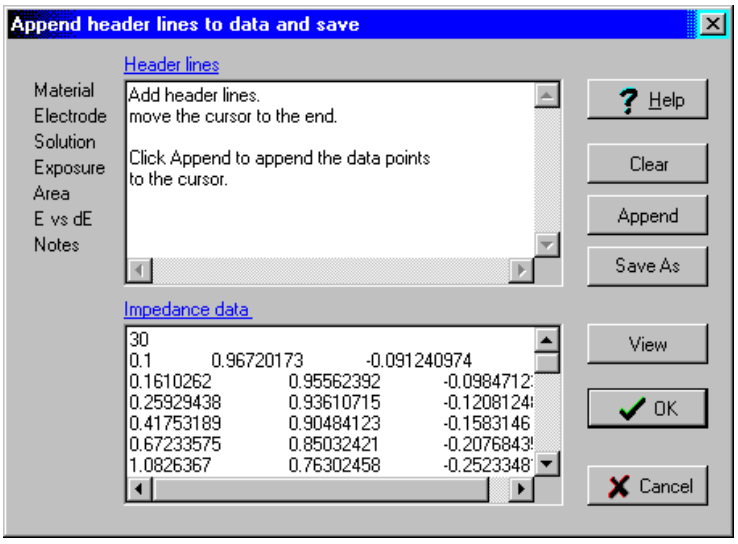
Create a new folder. Before data analysis, you can create two matching folders to store impedance data and to save computational results. For example, **...\data\plant data** and **...\par\plant par**.



Next topic: Append Header LInes

Append Header Lines

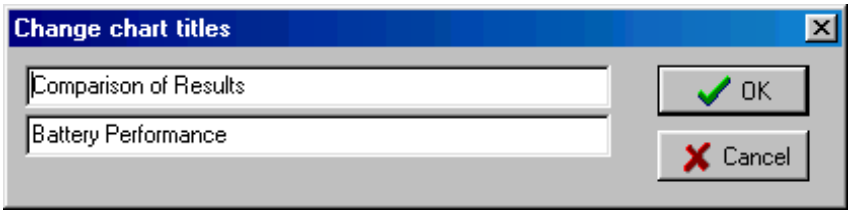
Impedance data can contain any number of header lines. Important information about the data can be appended.



Next topic: Edit Simulation Parameters

Change Chart Titles

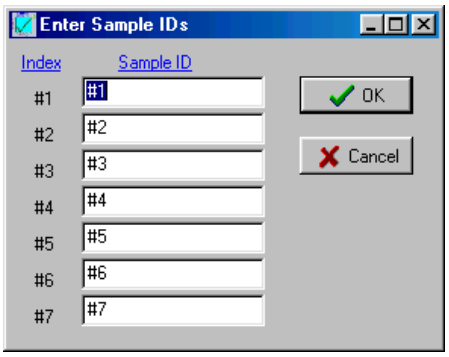
Two lines of chart titles can be changed before printing a plot.



Next topic: Edit Sample IDs

Edit Sample Ids

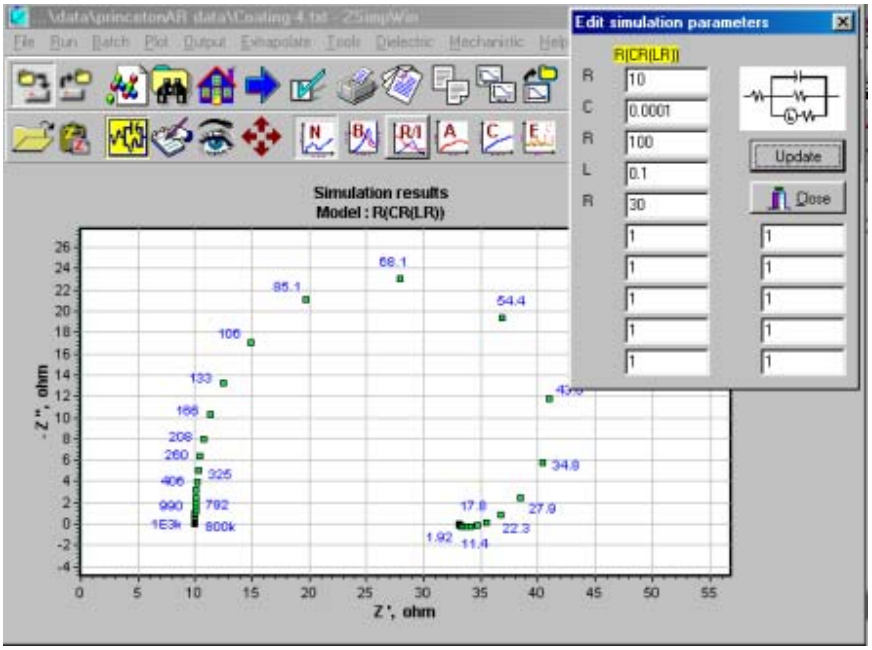
When multiple data sets are on a screen, it would be desirable to edit the sample IDs. Seven data sets can be placed in a plot.



Next topic: Edit Simulation Parameters

Edit Simulation Parameters

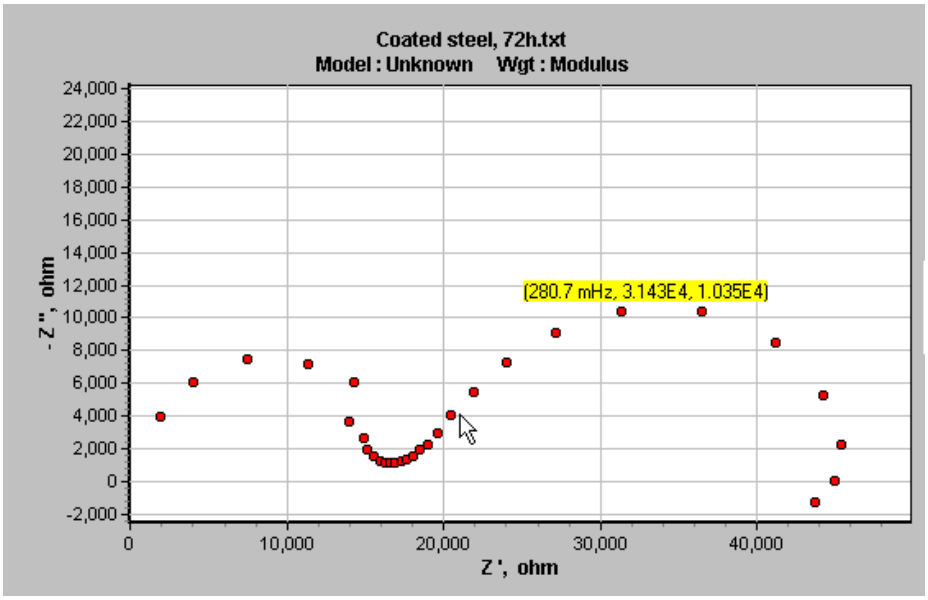
Allows easy change of the values of the parameters in **Simulate Mode**. Click on the **[Update]** button after changing any of the parameters.

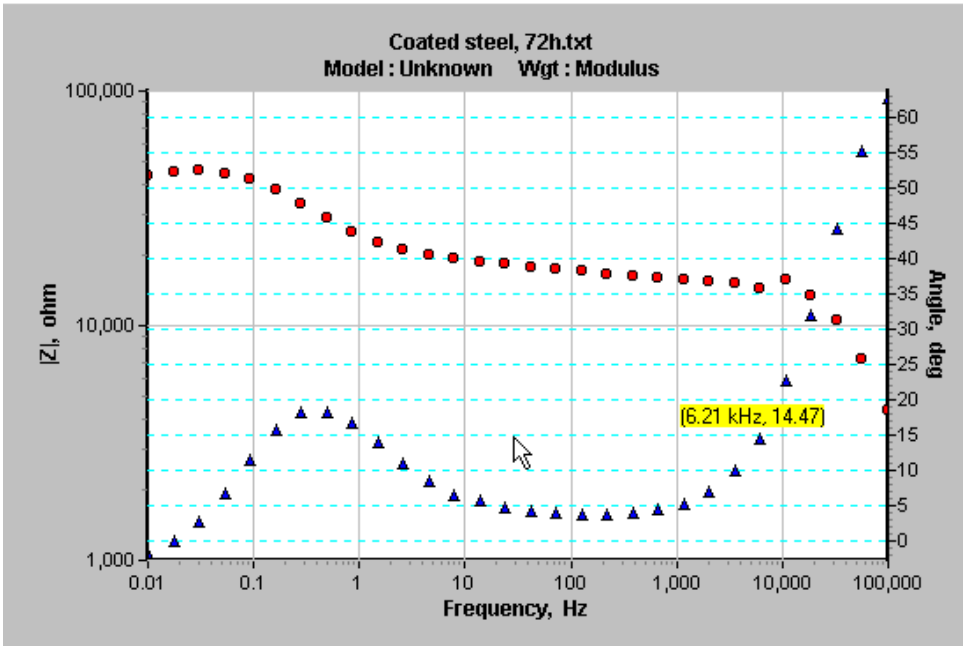


Next topic: Minihelp Screens

Reading the Coordinate of a Data Point

Locate a point and click the mouse button to read its coordinate. The coordinate is displayed in (frequency, real, imaginary) or (frequency, the variable in the vertical axis). The frequency is displayed in uHz, mHz, Hz, kHz, or MHz.





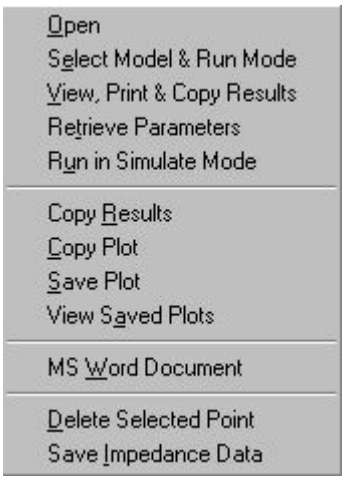
Next topic: Deleting Data Points

Deleting data points

Data points can be deleted and saved as a new file.

1. Move the mouse cursor to the point to delete and left-click to read its coordinate.
2. Right-click and select the "Delete Selected Point" from the Pop-up Menu.
3. Repeat deleting points.
4. Right-click and select the "Save Impedance Data" from the Pop-up Menu.

The new data file will be saved with the "*.dat" as the file extension and saved into the same folder. These two menus are present in the File Menu, however, it would be more convenient to access them from the Pop-up Menu.



Next topic: Close examination of a local area

Close examination of a local area

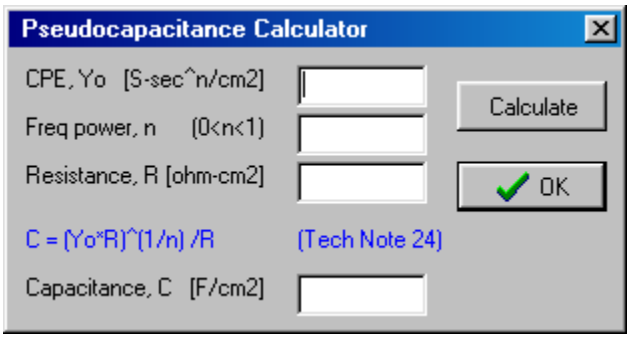
Focus an area
1. Click the bottom-left of a rectangle.
2. Drag diagonally to the top-right of the rectangle.
3. Release the mouse button.
4. Repeat the above procedure.

Reset
1. Click the top-right of a rectangle.
2. Drag diagonally to the bottom-right.
3. Release the mouse button.

Next topic: Minihelp Screens

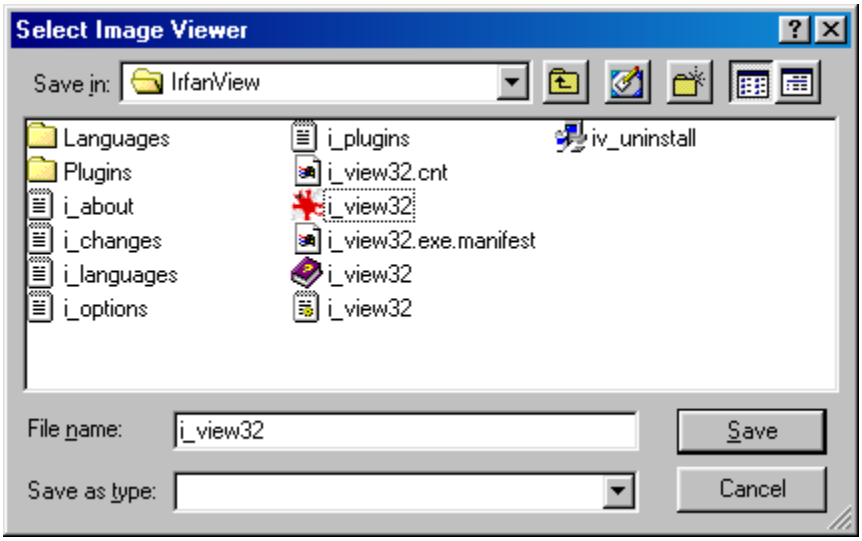
Get Pseudocapacitance

Computes the equivalent capacitance for a CPE by keeping the relaxation time constant associated with the CPE.



Specify Image Viewer

Specifies an image viewer installed on the computer. The name of the program and its location are stored. This program will be used to view saved plots in the current and later sessions.

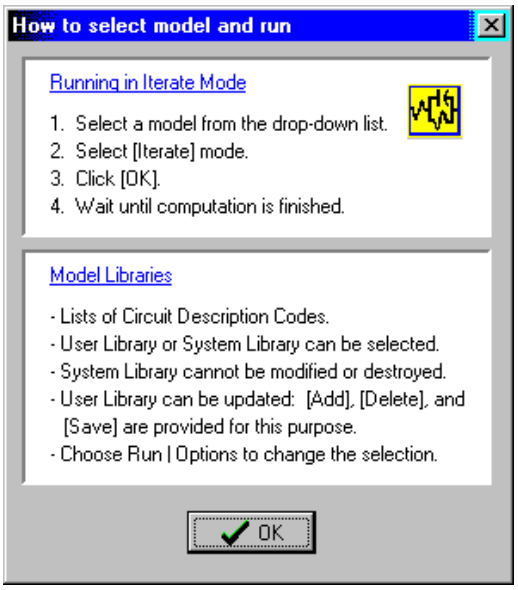


Minihelp Screens

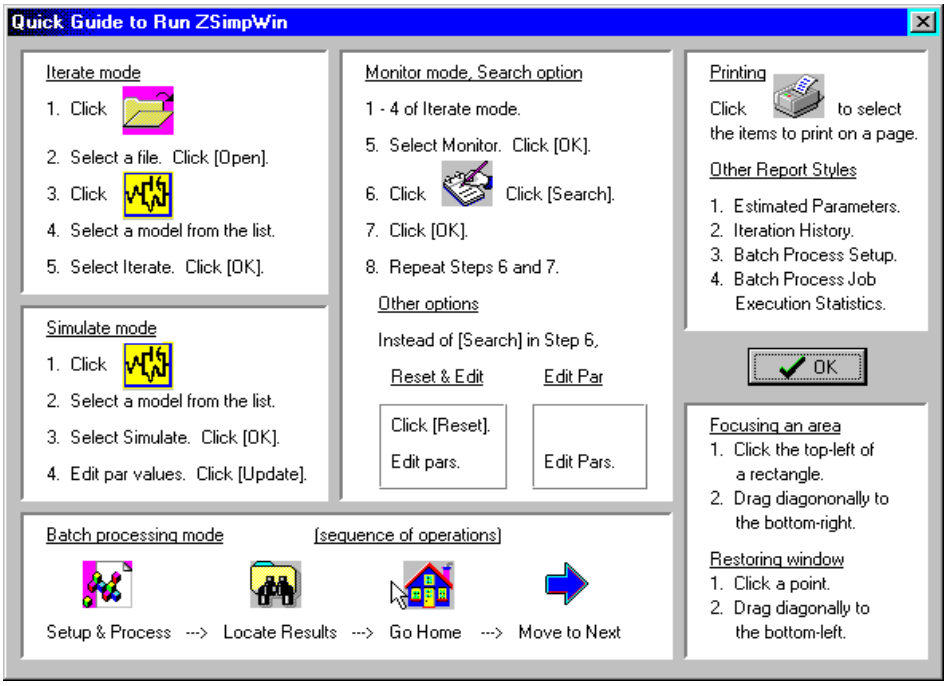
Minihelp screens are accessed by clicking the "Help" buttons in dialog screens.

- How to Run
- How to Select Model and Run Mode
- How to Edit and Run
- How to View, Print and Copy
- How to Change Options
- How to Paste Z Data
- How to Setup Batch and Run
- How to Show Tips
- How to Check Progress
- How to Print Project Group
- How to Prepare a Single-page Document
- How to Extrapolate
- How to append header lines

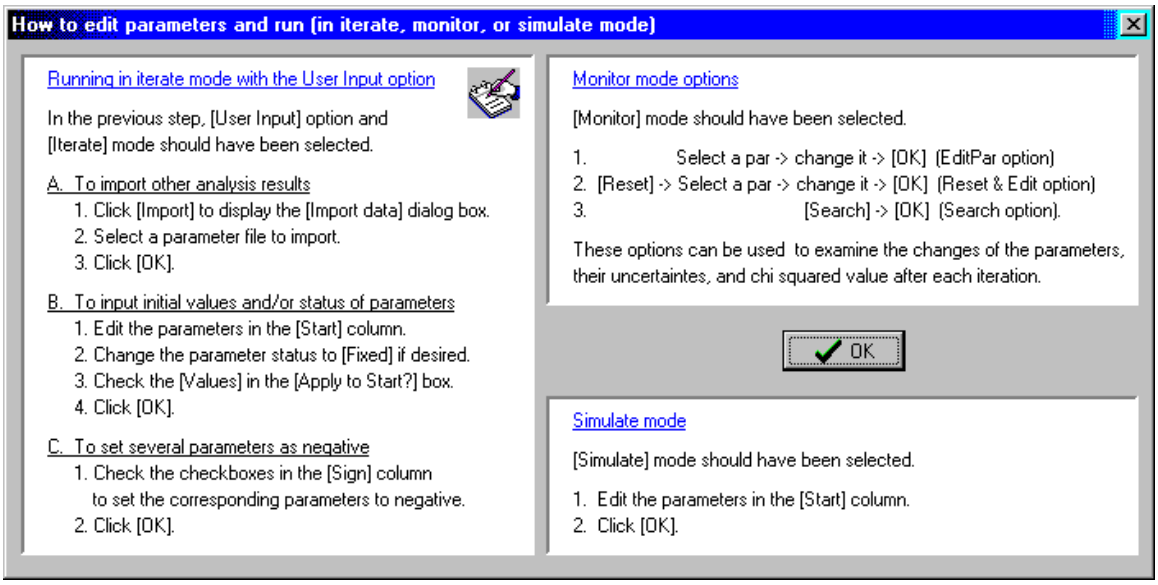
How to Select Model and Run Mode



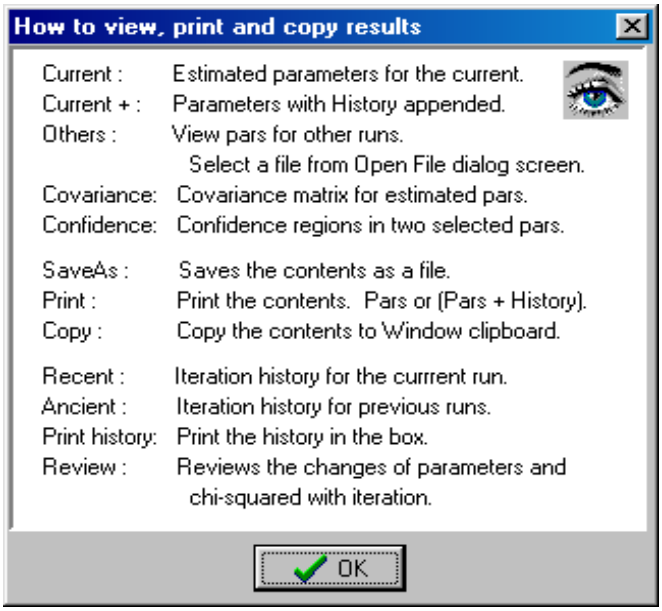
How to Run



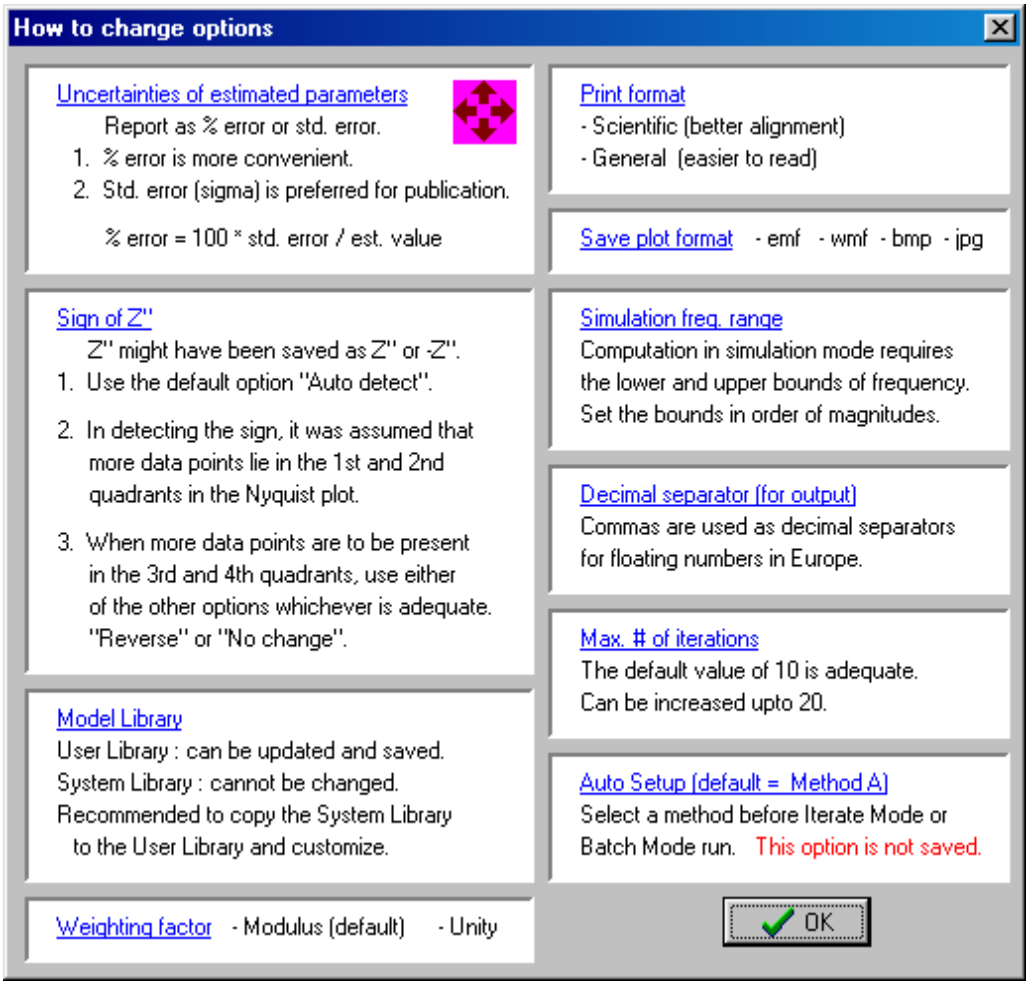
How to Edit and Run



How to View, Print & Copy Results

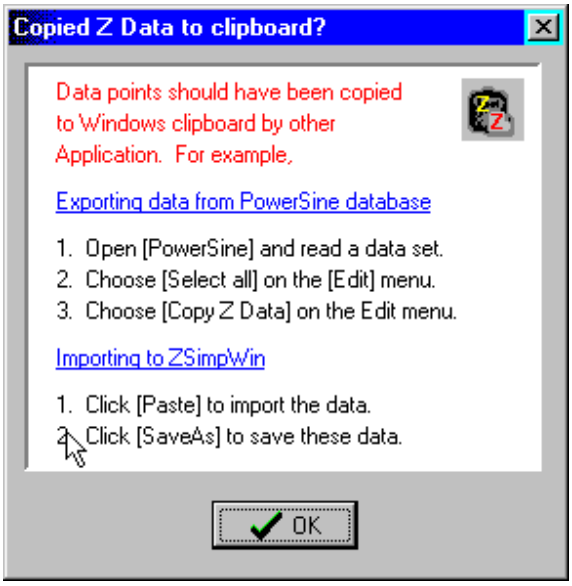


How to How to Change Options



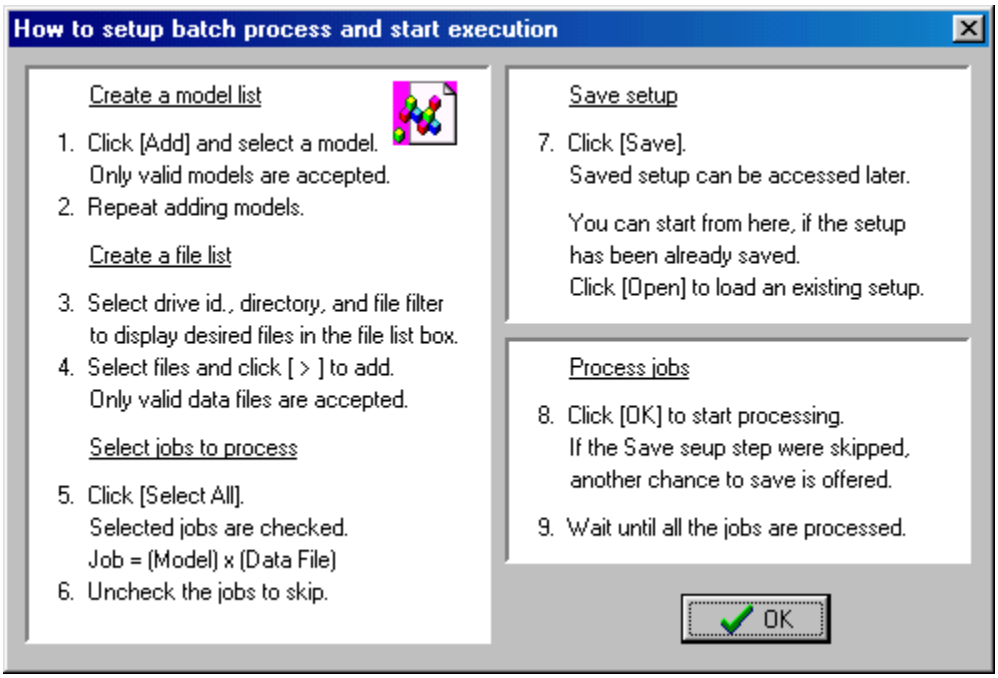
Next topic: How to Paste Z Data

How to Paste Z Data

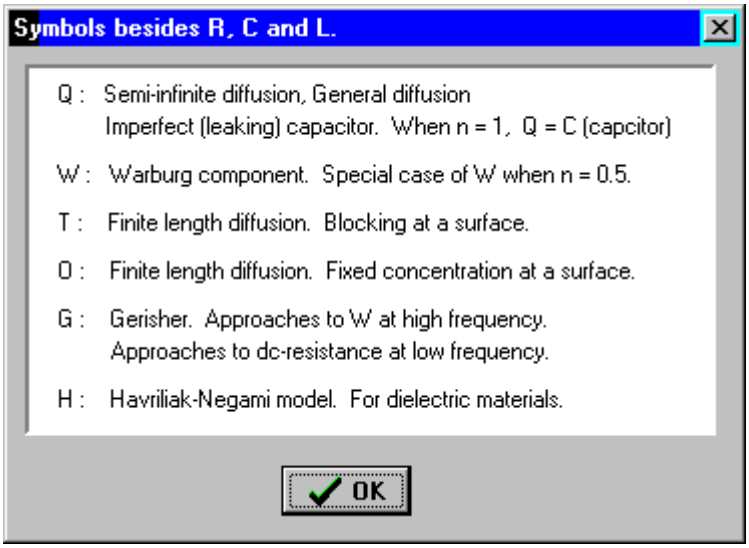


See Application Example 8.

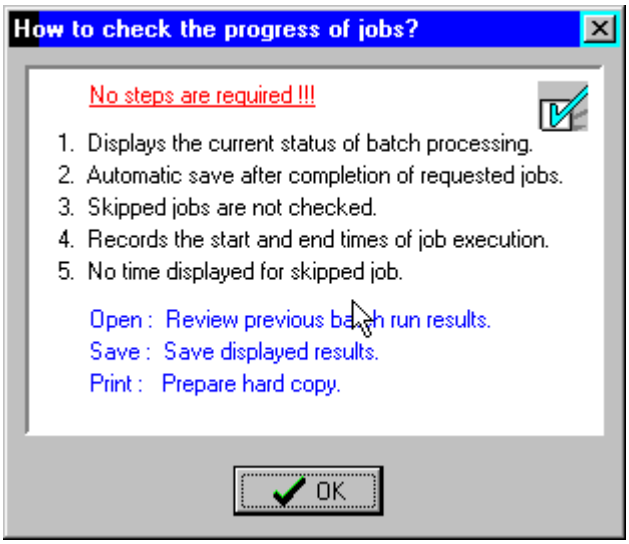
How to Setup Batch Process



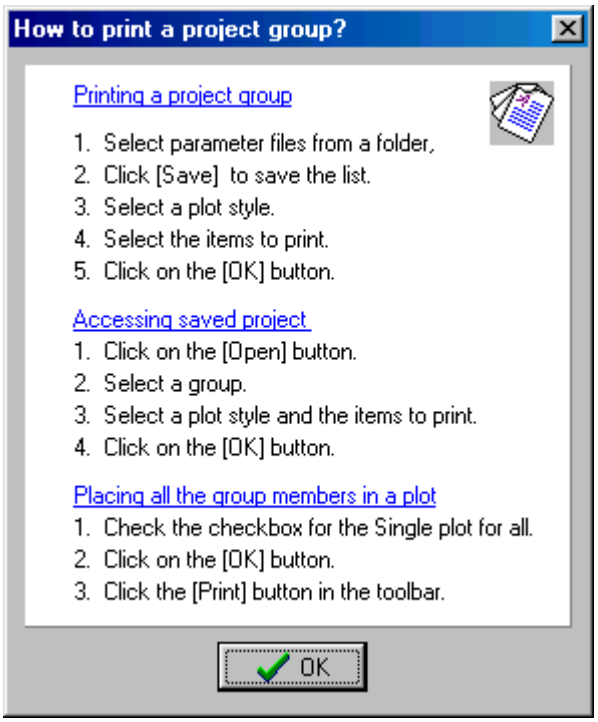
Show Tips



How to Check Progress

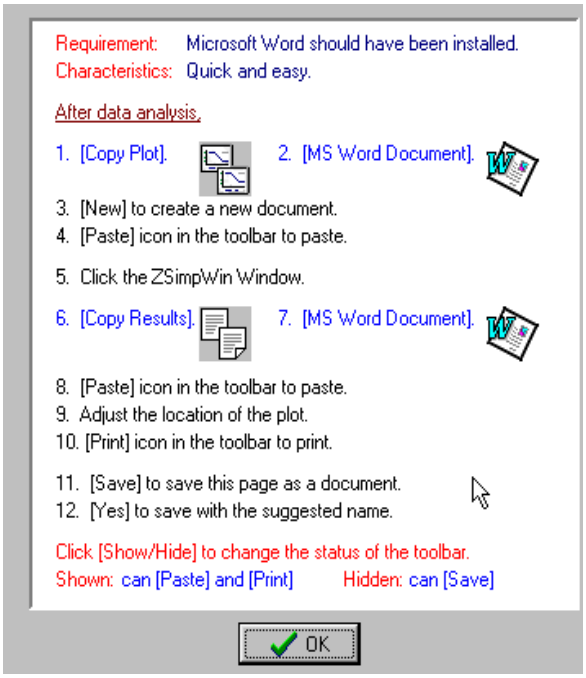


How to Print Project Group

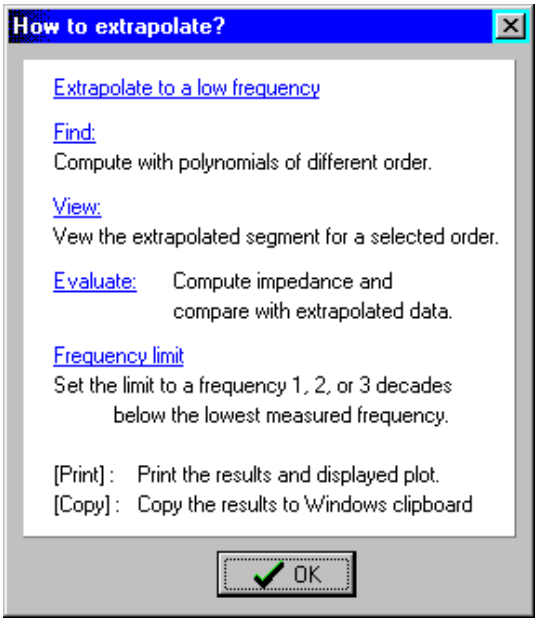


Next topic: How to Extrapolate

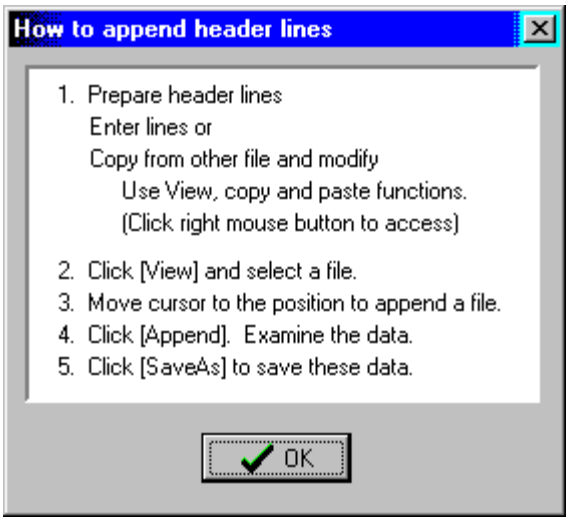
How to Prepare a Single-page Document



How to Extrapolate



How to append header lines



Operating instruction

This section describes basic operating instruction.

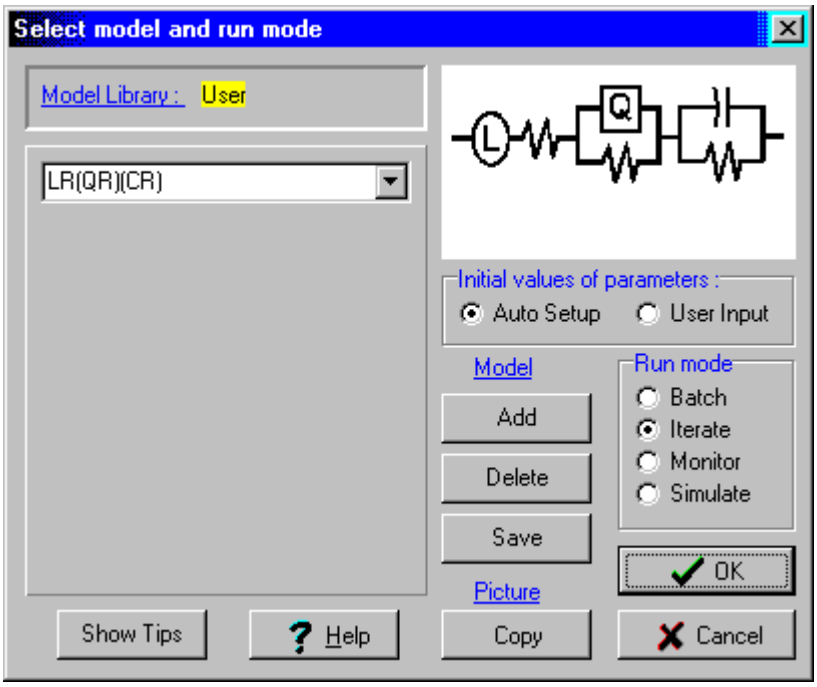
- **Running in Iterate mode**
- **Iterate mode with User input option**
- **Flowchart: Iterate mode run**
- **Batch mode**
- **Flowchart: Batch process setup**
- **Simulate mode**

Running in Iterate Mode

Iterate mode is the workhorse of ZsimpWin.

1. Click  to select a file. Navigate to the folder impedance data are stored by double-clicking each folder in the path until the **Look in** box displays the name of the desired folder. Select a file for analysis.

2. Click  .



3. Select a model. The drop-down list contains 75 models. Click the down-arrow to view the models in the list, move down to the desired model, and click to select it. The selected model will be displayed in the edit box with the corresponding picture displayed in the rectangle on the right. **Initial parameters** and **Run mode** options are set to **Auto Setup** and **Iterate** as default, respectively. If they have been changed from a previous run, reset these options.

4. Click **OK**.

5. Wait until computation is finished.

Next topic: Iterate Mode with User Input option

Iterate Mode with User Input Option

In an **Iterate mode** run with the **Auto Setup** option, it is assumed that all the parameters are positive and they are changed during iteration.

When should we use the User Input option?

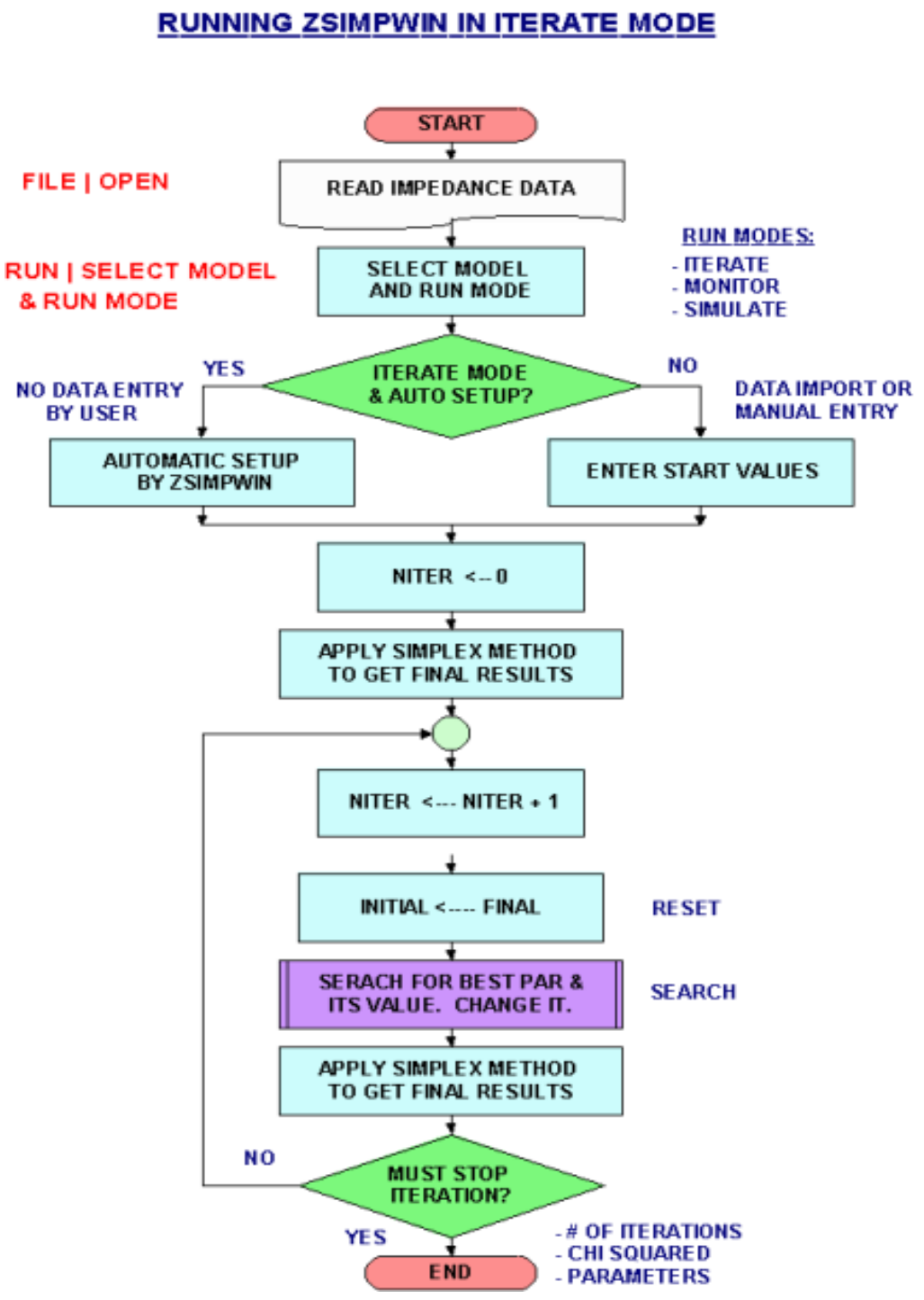
- To keep several parameters as constants: Set several parameters as constants before iteration. These parameters are not changed during data analysis.
- To specify several parameters as negative: See **Application Example B** in a separate document.

When can we use this option?

- To utilize analysis results of other data: Use import values as the initial guess of the parameters rather than the rough initial guess provided with the **Auto Setup** option. (See Example 5: Importing data).

Next topic: Running in batch processing mode

Flowchart, Iterate Mode Run



Next topic: Running in batch processing mode

Running in batch processing mode

A batch process consists of setup, running, and examination of analysis results. An auxiliary function is provided to check its progress.

Setup batch process and run
A batch contains multiple jobs each of which is defined by application of a model to a file. Setup starts with specifying several models and selecting files from a folder (**Input folder**). Total available jobs are the combinations of the models and the files. Jobs to be processed are selected by the user.

1. Create a model list
2. Create a file list
3. Select the jobs to be processed
4. Save the setup
5. Run

See Application Example 6

Review batch processing run results
Analysis results for each job are saved after a batch processing run. Locate and examine these results.

- Locate Results
- Go Home
- Move to Next

See Application Example 7

Check Progress
Displays the start and end times of each job. If a batch processing is on progress, the times of executed jobs and currently on progress are displayed.

See Check Progress

Next topic: Running in Simulate Mode

Running in Simulate mode

Computation is performed for a model and specified parameter values.

1. Click  .

2. Select a model from the drop-down list.

3. Set **Run mode** to **Simulate**.

4. Click **[OK]** in the **Select model and run mode** dialog box.

The **Edit Simulation Parameter** dialog box appears on the top-right corner of the screen (See Edit Simulation Parameters).

5. Enter the values of the parameters associated with the selected model in the edit boxes.

6. Click **[Update].**

See Application Example 9 .

Next topic: Application Examples

Application Examples

These examples serve as Tutorials for ZSimpWin. Start with Example 1 and 2 to learn about the key ingredients in ZSimpWin.

Application examples are as follows:

Iteration mode with Auto Setup option

- Example 1: Running in iterate mode
- Example 2: Viewing Results
- Example 3: Retrieving saved results
- Example 4: Keeping results for different sample areas.

Iteration mode with User Input option

- Example 5: Importing data

Batch processing

- Example 6: Setting up a batch process
- Example 7: Examination of batch process run results

Special cases

- Example 8: Pasting impedance data : reading PowerSine data
- Example 9: Running in simulate mode
- Example 10: Data for dielectric materials.

Summary of tests performed with included data

Models applied to sample data

Models applied to sample data

Sample ID	Ladder	Maxwell	Voigt	Note
Impedance data: **Estimated parameters:**	**...\data\princetonAR data** **...\par\princetonAR par**			
Battery-1	LR(Q(R(CR)))	LR(QR(CR))	LR(QR)(CR)	
Battery-2	LR(Q(R(CR)))	LR(QR(CR))	LR(QR)(CR)	
Battery-3	LR(Q(R(CR)))	LR(QR(CR))	LR(QR)(CR)	
Battery-4	LR(Q(R(CR)))	LR(QR(CR))	LR(QR)(CR)	Ex 1, 2, 3
Virgin coating-1 Virgin coating-2 Virgin coating-3 Virgin coating-4	R(CR) R(CR) R(CR) R(CR)			Ex 6, 7 Ex 6, 7 Ex 6, 7 Ex 6, 7
Coating-1	R(C(R(CR)))	R(CR(CR))	R(CR)(CR)	
Coating-2	R(Q(R(Q(R(CR)))))	R(QR(QR)(CR))	R(QR)(QR)(CR)	
Coating-3	R(Q(R(Q(R(Q(R(CR)))))))	R(QR(QR)(QR)(CR))		Ex 5
Coating-4	R(C(R(Q(RW))))	R(CRQ(RW))		Ex 5
Cylinder in NaCl	LR(QR)			
Steel, initial	LR(C(R(Q(R(C(RW))))))	LR(CR(QR)(RW))		
Steel, 72h	R(Q(R(QR)))	R(QR(QR))	R(QR)(QR)	
Coated steel, init	LR(C(R(Q(R(LR)(CR)))))			Poor fit
Coated steel, 64h	LR(C(R(Q(R(LR)(CR)))))	LR(CR(QR)(LR)(CR))		
Coated steel, 72h	R(C(R(Q(R(LR)(CR)))))	R(CR(QR(LR)(CR))		
Pd_md15s	R(C(R(CR)))	R(CR(CR))	R(CR)(CR)	
Pd_md30s	R(C(R(CR)))	R(CR(CR))	R(CR)(CR)	Ex 8
Pd_md60s	R(C(R(CR)))	R(CR(CR))	R(CR)(CR)	
Impedance data: **Estimated parameters:**	**...\data** **...\par**			
Cu_Ni exposed to sea water	R(Q(R(QR)))	R(QR(QR))		Ex 4
HN Saved as Z Data	(HC)			Ex 10

Impedance data: **Estimated parameters:**	**...\data\simulation data** **...\par\simulation par**			
LR(CR).sim and LR(CR).par	LR(CR)			Ex 9
Impedance data: **Estimated parameters:**	**...\data\boukamp data** **...\par\boukamp par**			
Oxygen ion conducting	LR(C(R(QR)))	LR(CR(QR))	LR(CR)(QR)	Ex A-1
Oxygen ion conducting		LR(C(QR))	LR(CR)Q	Ex A-1
Porous gold electrode	LR(Q(R(C(R(LR)(CR)))))	LR(QR(CR)(LR)(CR))		Ex A-2
Porous gold electrode	LR(Q(R(LR)(CR)))	LR(QR(LR)(CR))		Ex A-2
Passivation of chromium		R(QR(OR))		Ex B
Passivation of chromium		R(QR(CR)(OR))		Ex B
Impedance data: **Estimated parameters:**	**...\data\boukamp data** **...\par\boukamp par**			
Concrete_1		R(CR(QR))		
Concrete_2		R(CR(QR)(OR))		
Cu_Ni Sample B	R(Q(R(C(R(C(RW))))))(CR)	R(QR(CR)(RW))(CR)		
P211p20	R(C(R(Q(R(QR)))))	R(CR(QR)(QR))		

Example 1: Running in Iterate Mode

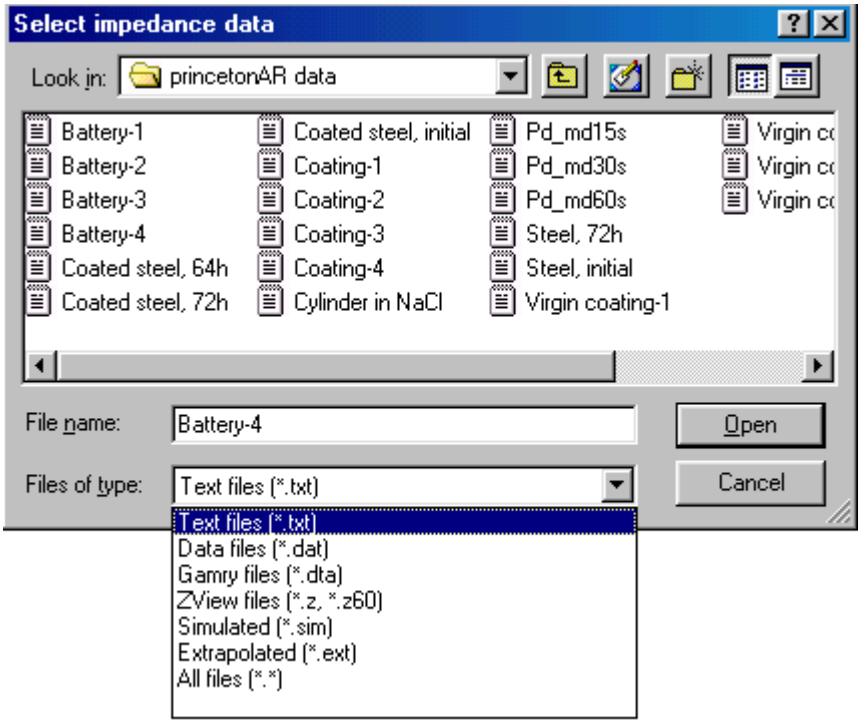
Modeled **...\data\princetonAR data\Battery-4.txt** with **LR(QR)(CR)**. Operating procedure?

Solution

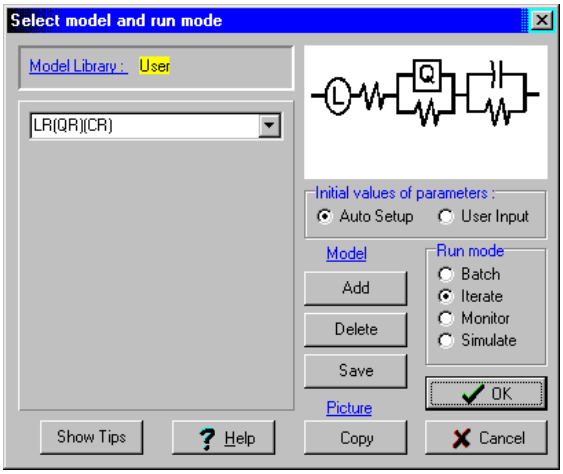
This is the work horse of ZsimpWin. Desirable solution is obtained by running in iteration mode with **Auto Setup** option in most situations.

Procedure

1. Click  to bring up the **Select impedance data** dialog box. Navigate to the folder **...\data\princetonAR data** by double-clicking each folder in this path until the **Look in** box displays the **princetonAR data** folder. Select the file **Battery-4** and click **[Open]**.



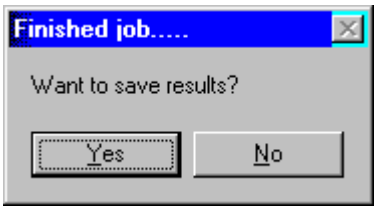
2. Click  . Click the drop-down button to expose the models in the drop-down list and choose **LR(QR)(CR)**. **Initial parameters** and **Run mode** options are set to **Auto Setup** and **Iterate** as default. If they have been changed from a previous run, reset these options.



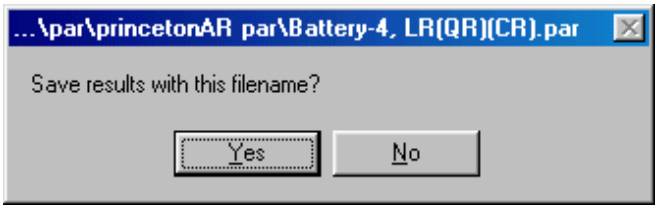
3. Click **[OK]**.

4. A small **Please wait...** dialog box appears at the top-left corner of the screen. This indicates the progress of computation. Wait until computation is finished.

5. At the end of the computation, you are asked whether to save the results. Click **[Yes]**.



6. A save filename is suggested. Click **[Yes]**.



Next topic: Application 2: Viewing Results

Example 2: Viewing results

Results obtained after running Application Example 1 consist of the following three data files:

Parameters: ... \par\princetonAR par\Battery-4, LR(QR)(CR).par
Iteration History: ... \hist\Battery-4, LR(QR)(CR).hst
Variation of parameters: ... \temp\ Battery-4, LR(QR)(CR).mat

A plot or a text file can be displayed first before printing. Click a plot style speed button (Nyquist, Bode, Real and Imag, Admittance, or Capacitance) in the main Window to change the style of the displayed plot. Perform the following exercises (in no particular order) to learn about printing results in various formats.

In the main Window,

1. Click  to print estimated parameters and displayed plot on a single page (See Print Item Selection).
2. Click  to copy the plot to Windows clipboard. This content can be pasted to other documents. For example, open Microsoft Word. Choose **New** on the **File** menu. Choose " **Paste** on the **Edit** menu. Plot will be pasted to the new document.

Click  to display **View, print & copy results** dialog box. The files corresponding to the current run are automatically displayed in two viewing areas. One is for parameters and the other is for iteration history. The iteration history shows the variation of the chi squared with iterations and the start and end times of each iteration.

See also:

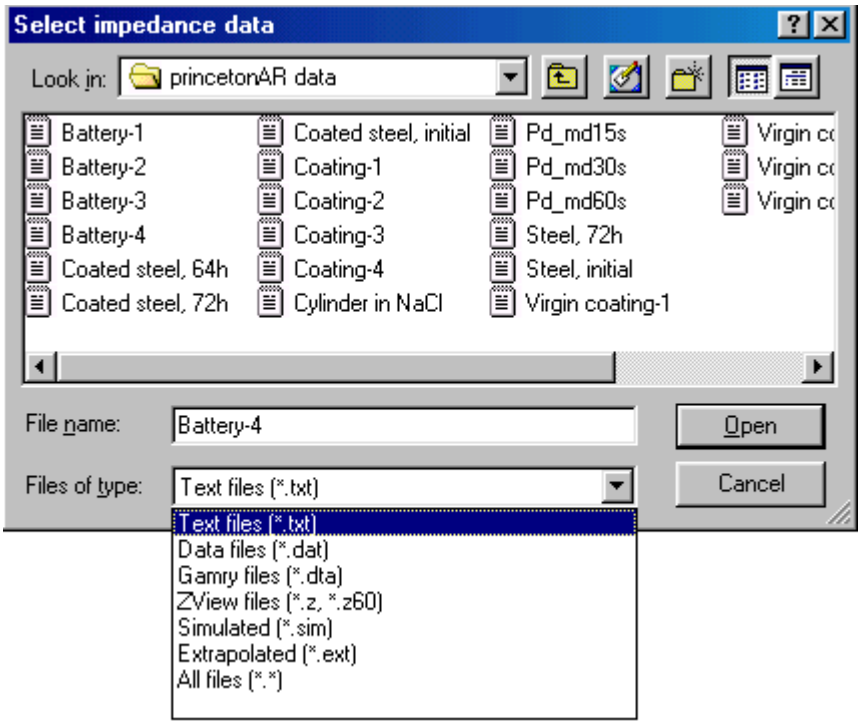
- View, Print & Copy Results.
- Estimated parameters
- Iteration History

Next topic: Example 3

Example 3: Retrieving saved results

Analysis results saved in previous sessions are accessed by following this procedure:

1. Click  to bring up the **Select impedance data** dialog box. Navigate to the folder **...\data\princetonAR data** by double-clicking each folder in this path until the **Look in** box displays the **princetonAR data** folder. Select **Battery-4** and click **[Open]**.



2. Click  to bring up the **Retrieve parameters** dialog box.

3. Navigate to the folder **...\par\princetonAR par** by double-clicking each folder in this path until the **Look in** box displays the **princetonAR par** folder.

4. Click **Battery-4** and click **[Open].**

You can view the analysis results following the procedure described in Example 2.

Note:

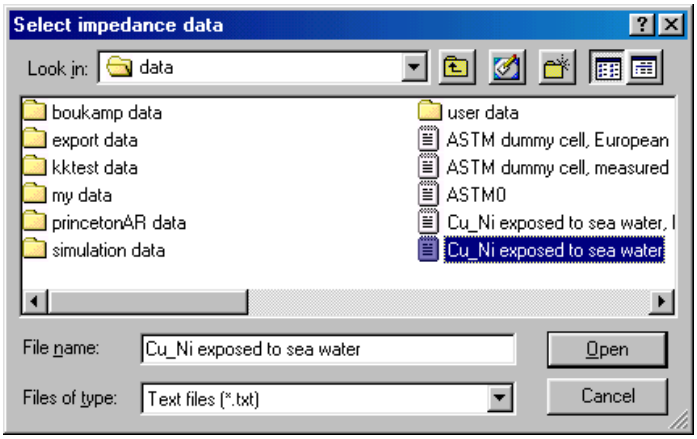
- More than 50 sample run results are included.
- Load and examine these results following the above procedure.

Example 4: Keeping results for different sample areas

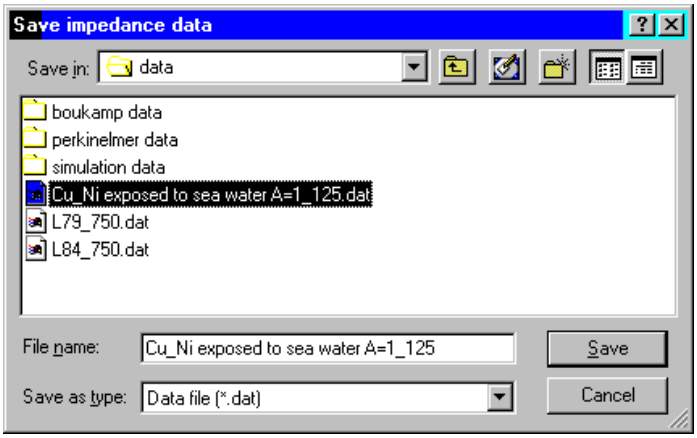
The data **Cu_Ni exposed to sea water.txt** were modeled with **R(Q(R(QR)))**. How can I save results for different sample areas (1cm2 and 1.125 cm2)?

It is recommended to create a data file by copying the data.

1. Click  to bring up the **Select impedance data** dialog box. Select the file and click **[Open]**.

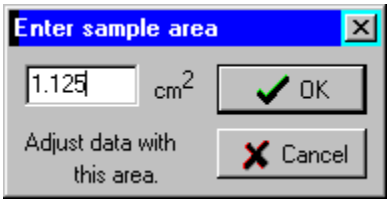


2. Choose **Save Impedance Data** on the **File** menu.



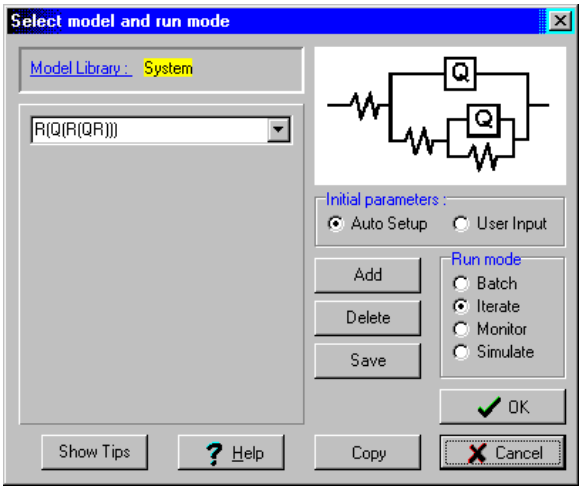
3. Type **Cu_Ni exposed to sea water A=1_125** in the filename field. Do not use period (".") in the file name. To indicate the area, **A=1_125** was added to the file name. Click **[Save]**.

4. Click **Sample Area** in the main window to display the **Enter sample area** dialog box. Change the area in the edit box to 1.125 cm2. Click **[OK]**.



5. Click  . Click the drop-down button to expose the models in the drop-down list and choose **R(Q(R(QR)))**.

6. Click **[OK]**.



7. Wait until computation is finished. Optimization results are saved in the **...\par\Cu_Ni exposed to sea water A=1_125, R(Q(R(QR))).par**, and the iteration history in **...\hist\Cu_Ni exposed to sea water A=1_125, R(Q(R(QR))).hst**.

Next topic: Example 5

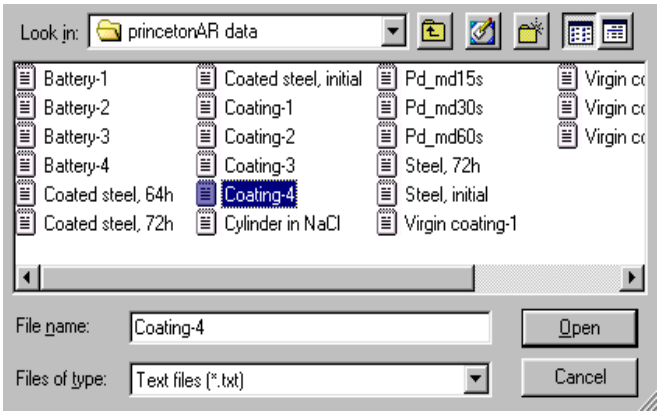
Example 5: Importing data

The data **Coating-4.txt** were modeled with **R(C(R(Q(RW))))**. Results for similar data have been obtained using the same model. Can I utilize these results?

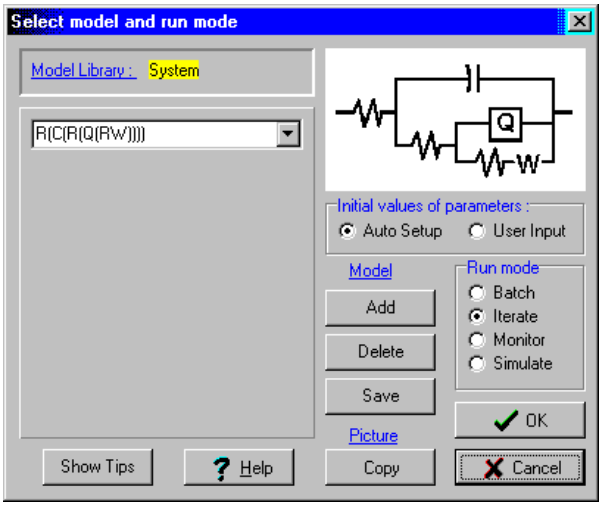
Available data
Data : ...\data\princetonAR data\Coating-4.txt
Results : ...\par\princetonAR par\Coating-3, R(C(R(Q(RW)))).par

Solution
You can compute using the default option (**Auto Setup**). For a higher computational efficiency, final results for similar data can be imported. Because the start values are closer to the true solution, the solution would be obtained in much less time.

1. Click  to bring up the **Select impedance data** dialog box. Navigate to the folder **...\data\princetonAR data** by double-clicking each folder in this path until the **Look in** box displays the **princetonAR data** folder. Select the file **Coating-4** and click **[Open]**.



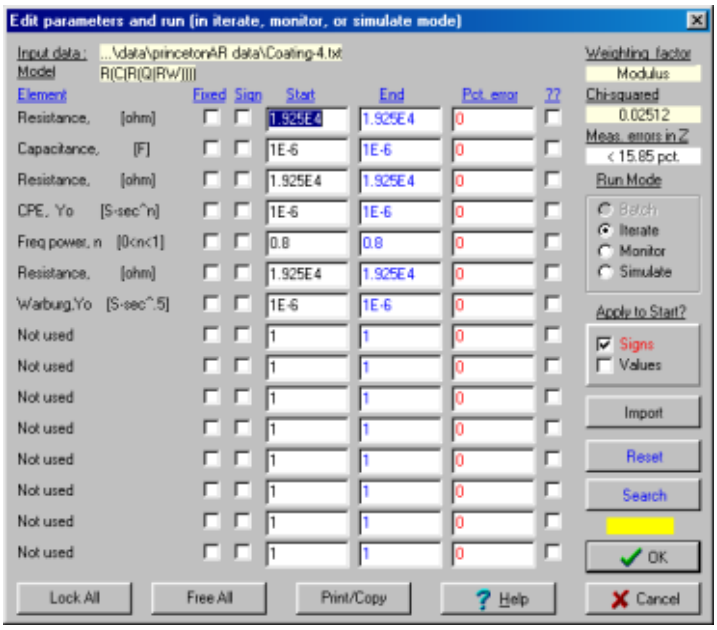
2. Click  . Click the drop-down button to expose the models in the drop-down list and choose **R(C(R(Q(RW))))**.



3. Change the **Initial parameters** option to **User Input**. Make sure **Run mode** is set to **Iterate**.

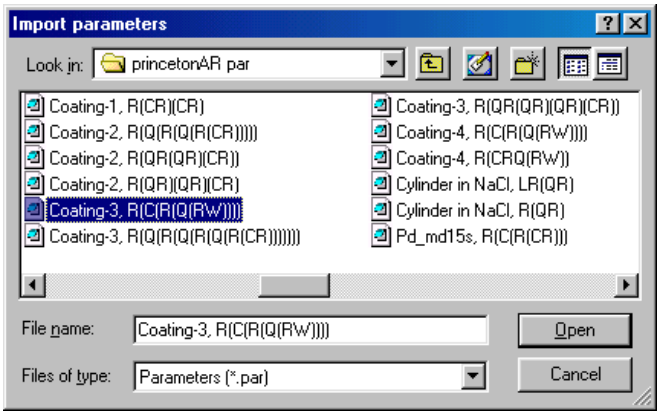
4. Click **[OK]**.

View, Edit & Run dialog box appears requesting input.

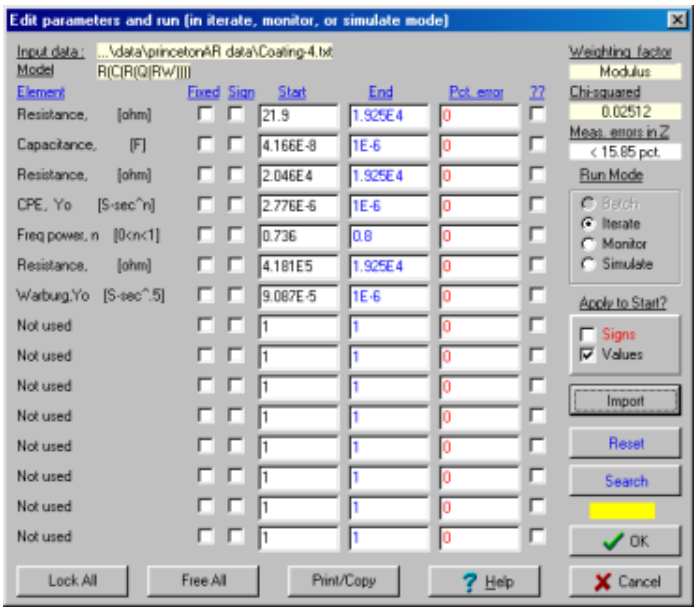


5. Click **[Import]** to display the **Import parameters** dialog box.

6. Select the parameter file **...\par\princetonAR par\Coating-3. R(C(R(Q(RW))))).par** and click **[Open]**.



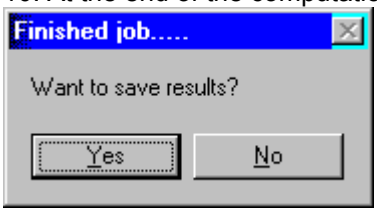
7. The values of the parameters are copied to the edit boxes in the **start** column. The checkbox **Values** in the **Apply to Start?** group is checked after this operation.



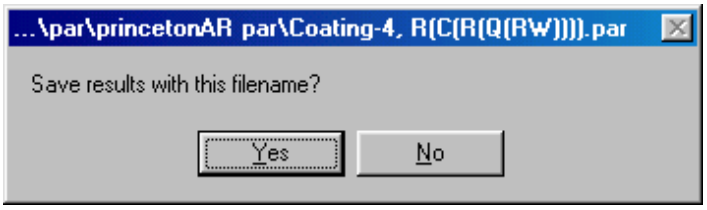
8. Click **[OK]**.

9. Wait until computation is finished. Iteration starts with the imported values of the parameters. The imported values are much better than the rough initial guess provided with the **Auto Setup** option.

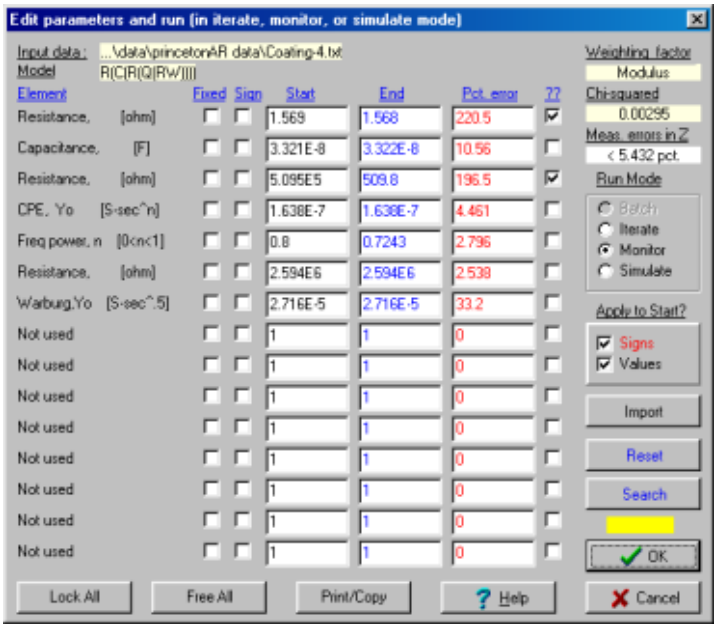
10. At the end of the computation, you are asked whether to save the results. Click **[Yes]**.

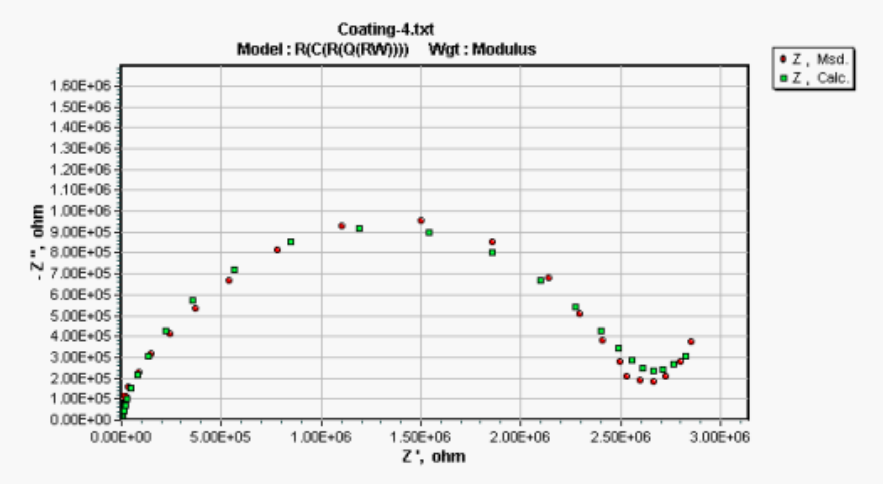


11. A save filename is suggested. Click **[Yes]**.



Final results:





Next topic: Example 6

Example 6: Setup batch process

Each job is defined by application of a model to a data file. A batch process consists of execution of multiples jobs in sequence. Define available jobs by creating a model list (several models) and file list (file names). Jobs are the combinations of the models and files. Select all of them as a batch. In practice some of the jobs are undesirable to execute. Remove undesirable jobs.

Available data:
...\data\princetonAR data\Virgin coating-1.txt
...\data\princetonAR data\Virgin coating-2.txt
...\data\princetonAR data\Virgin coating-3.txt
...\data\princetonAR data\Virgin coating-4.txt

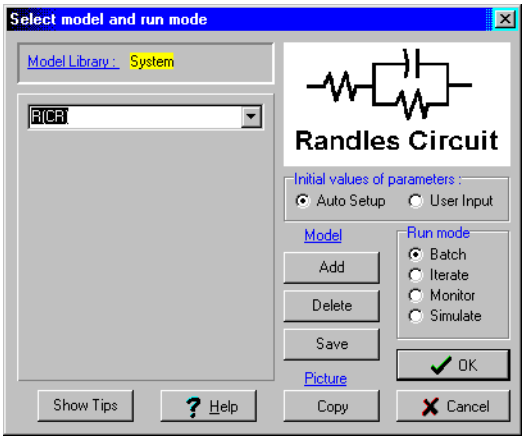
Applied Model: R(CR)

Conditions:
Skip computation for "**Virgin coating-3.txt**".
Save results in **...\par\princetonAR par** folder

Solution

This is the most complex procedure in ZsimpWin. Click  to show the **Setup batch process and start...** dialog box.

1. Click **[Add]** to grab a model.
2. The dialog screen used to select a model and run mode appears. Select **R(CR)** from the drop-down list and click **[OK].**

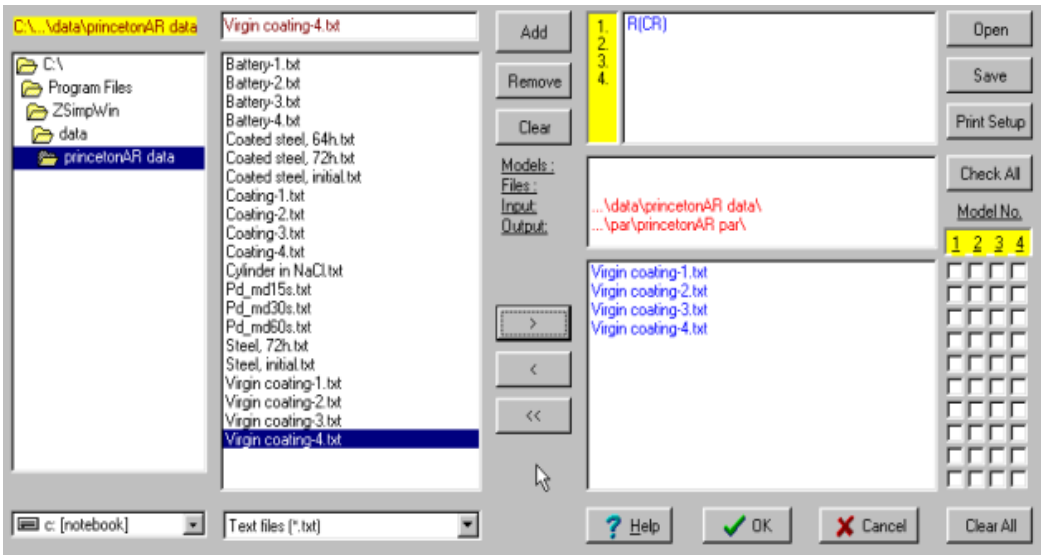


2. Add more models following the same procedure. The **[Remove]** is to remove a selected model and the **[Clear]** is to clear the model list by removing all the models.

3. Select Drive id, File directory, and File Filter. Display only the files of interest in the file list box.

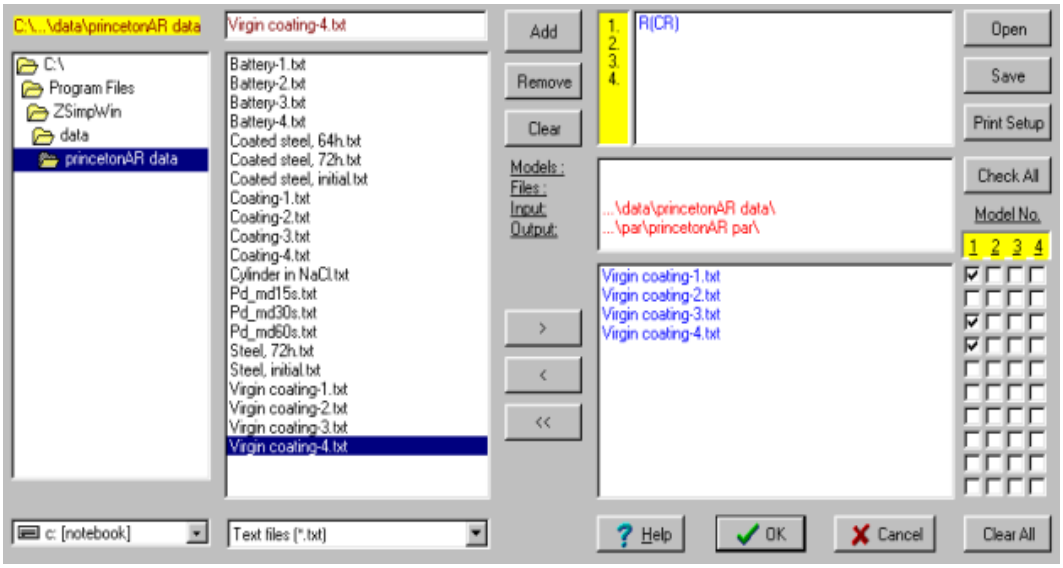
4. Select a file and click the **[>]** to add to the file list.

5. Select more files and add to the list. Add four files from the **...\data\princetonAR data**. The **[<]** and **[<<]** are to remove a selected file and clear all the files, respectively.

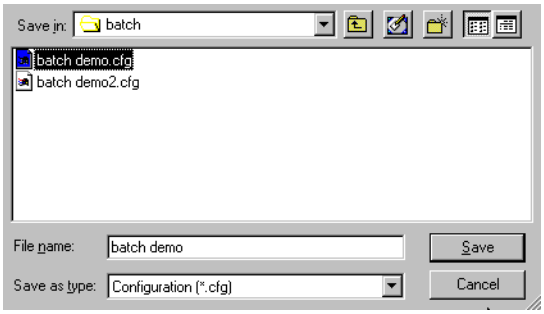


6. All the files are added from the same folder. This will facilitate organizing a group of files. Input and Output folders are **...\data\princetonAR data** and **...\par\princetonAR par**, respectively. Results are saved in the Output folder.

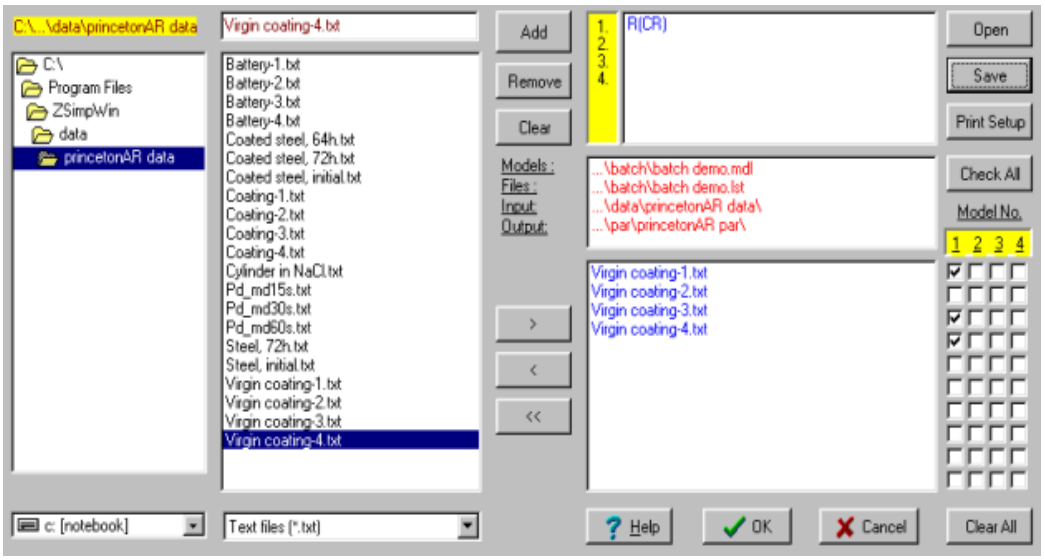
7. Check boxes are associated with jobs. Click **[Check All]** to include all the available jobs into the batch. Because one model is applied to four files, four boxes will be checked. To skip the third job. Uncheck the checked box.



8. This is the setup you have prepared, however, not been saved. The names of the model list and file list are still vacant. Click **[Save]** to save this work. The **Save batch processing setup** dialog box will appear requesting your input. Type "**batch demo"** in the **file name** edit field.



9. Now the model list and file list are saved as **...\batch\batch demo.mdl** and **...\batch\batch demo.lst**, respectively. The file **...\batch\batch demo.cfg** specifies the batch with the four lines displayed on the dialog.



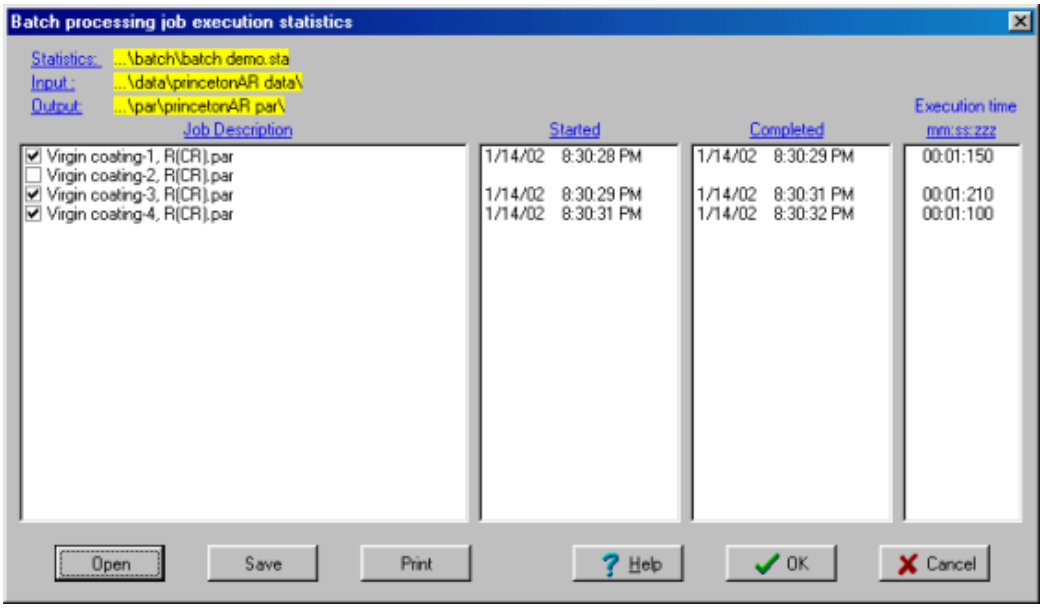
10. Note that additional information should have been saved, i.e., the check status of the check boxes. When the **[Save]** is clicked, the check status is also saved as **...\batch\batch demo.tmp**.

11. When you want to access the setup file in a later session, click **[Open]** to grab all the data about configuration displayed in the dialog box. **Open batch processing setup** dialog box appears. Select the configuration file and click [**Open]**. Click **[Print]** to make a hard copy of the report showing **Batch Setup Specification** (See Batch process setup records).

12. Now click **[OK]** to start processing.

13. Wait until all the jobs are executed.

14. At the end of the execution, **Batch processing job execution statistics** dialog box is displayed on the screen. These records have been already saved in **...\batch\batch demo.sta** file. Click **[Print]** to print this report.



Next topic: Example 7

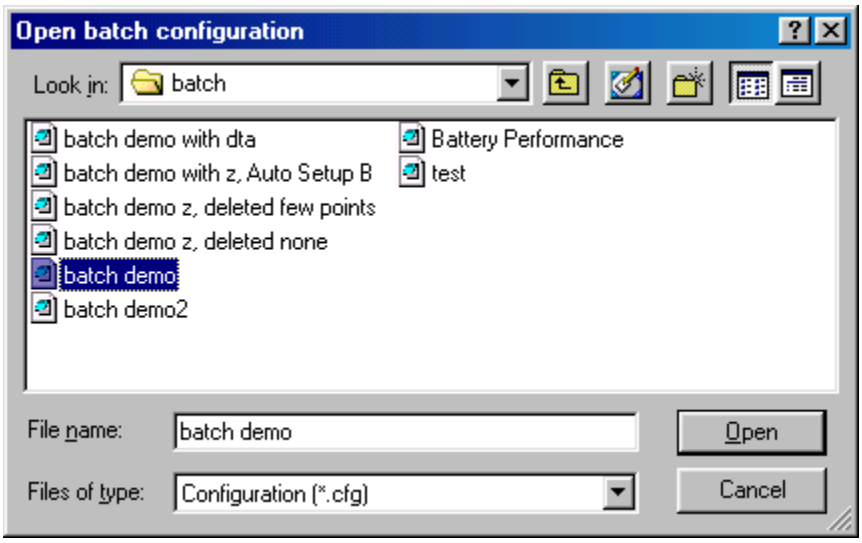
Example 7: Examination of batch process run results

Examine the analysis results saved after running **Example 6**. Four speed buttons are assigned for this purpose.

1. Click  to bring up the **Open batch configuration** dialog box.

2. Navigate to the folder **...\batch** by double-clicking the **batch** folder. The **Look in** box must display the **batch** folder.

3. Click **batch demo** and click **[Open]**.



4. Click  to go to the first job. All the results and parameters are available. Common View, Print and Copy functions (See Example 2) are available.

5. Click  to view the results for the next job. If a job was skipped, **"Skipped a job, Go to Next"** will appear on the screen.

6. **Batch processing job execution statistics** dialog box is also used to check the progress of jobs. When batch processing is requested, job name and selection status (selected or not) for all the jobs are recorded immediately, and the start and end times are recorded later one by one. Click the  on the main window to check the current status.

Note:
Three batch configurations, **batch demo**, **batch demo2,** and **batch demo3** are included.
Examine **batch demo2** following the above procedure.

Next topic: Example 8

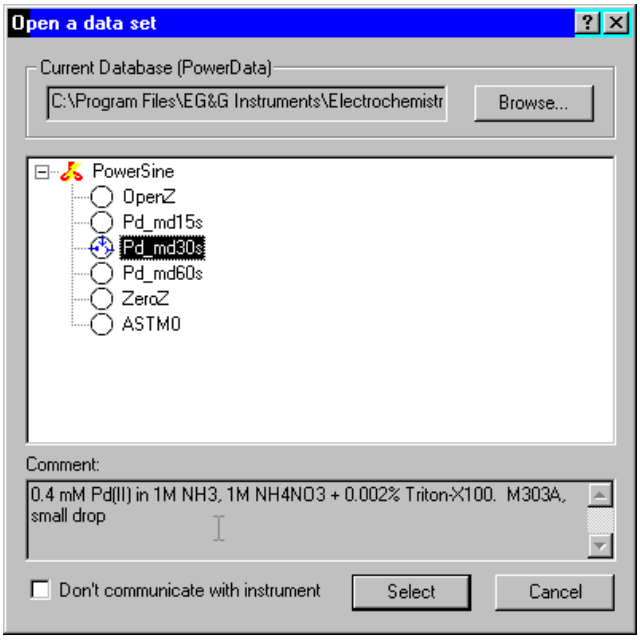
Example 8: Pasting Z Data from PowerSine

Available data: Pd_md30s in PowerSine Database.

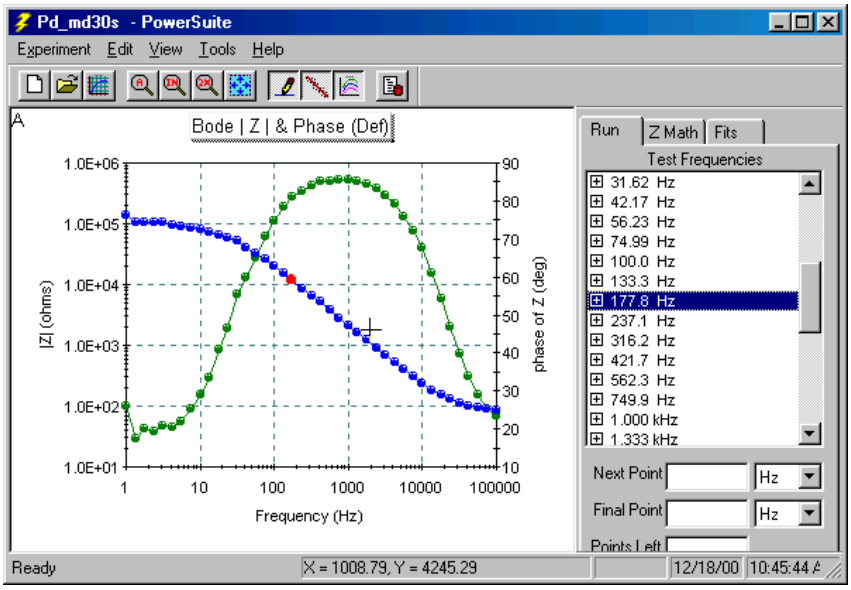
Procedure

1. Open **PowerSine** (See About PowerSine).

2. Choose **Open PowerSine** on the **Experiment** menu.

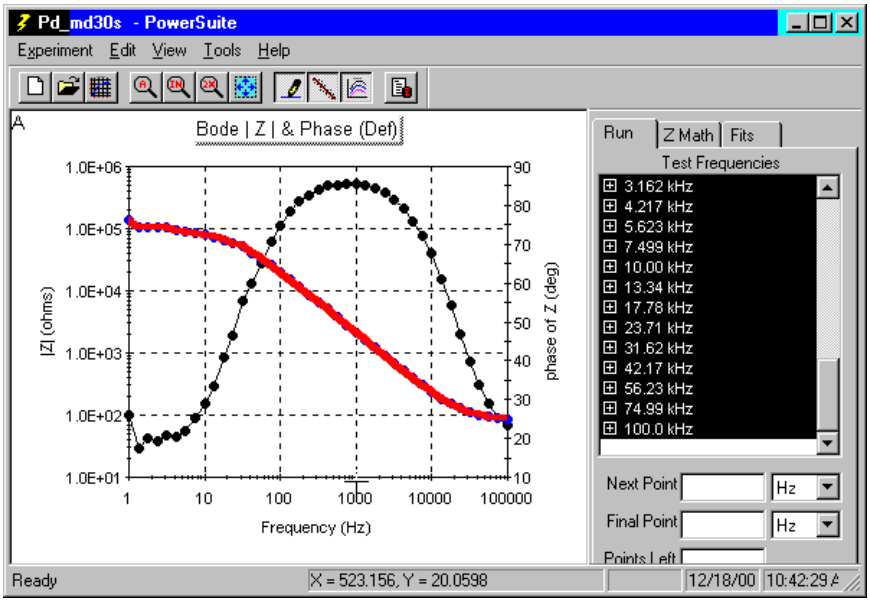


3. Click **PowerSine** to display the files in the database, select **Pd_md30s** and then click **[Select]**.



4. Choose **Select all** on the **Edit** menu to select all the data points

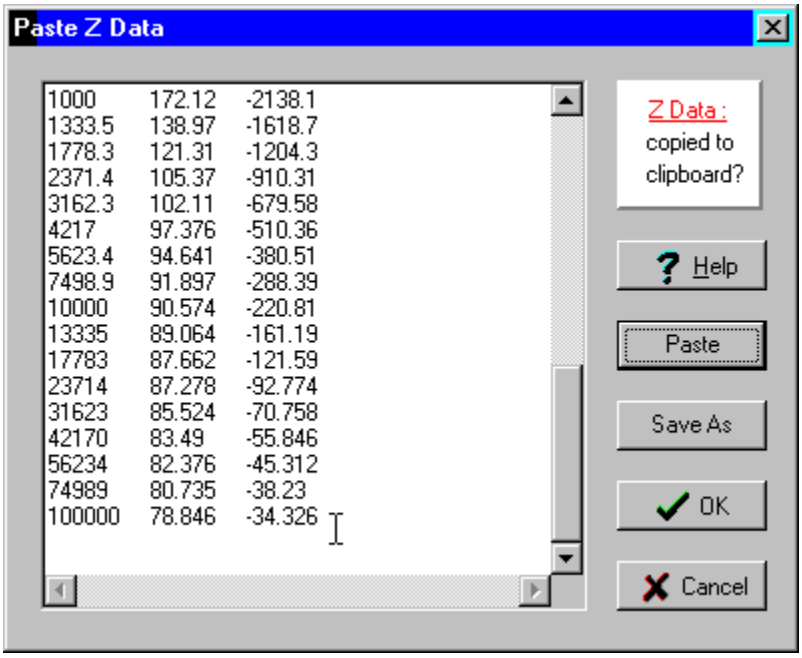
5. Choose **Copy Z Data** on the **Edit** menu to copy the selected data points to Windows clipboard.



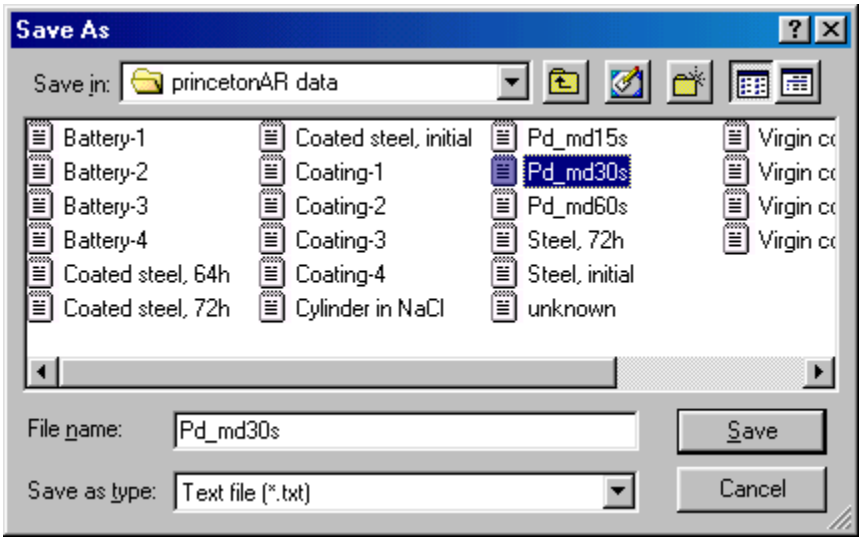
6. Open **ZsimpWin** at the Desktop (might have been opened already).

7. Click  .

8. Click **[Paste].**



9. Click **[SaveAs]** to display the **Save As** dialog box. Select the folder **...\data\princetonAR data** and type **Pd_md30s.txt** in the file name edit box.



Next topic: Example 9

Example 9: Running in Simulate Mode

See the curve for the Model **R1(C2R3(L4R5))** with R1=10 ohms, C2 = 1e-4 F, R3 = 100 ohms, L4 = 0.1 Henri, R5 = 30 ohms.

Solution

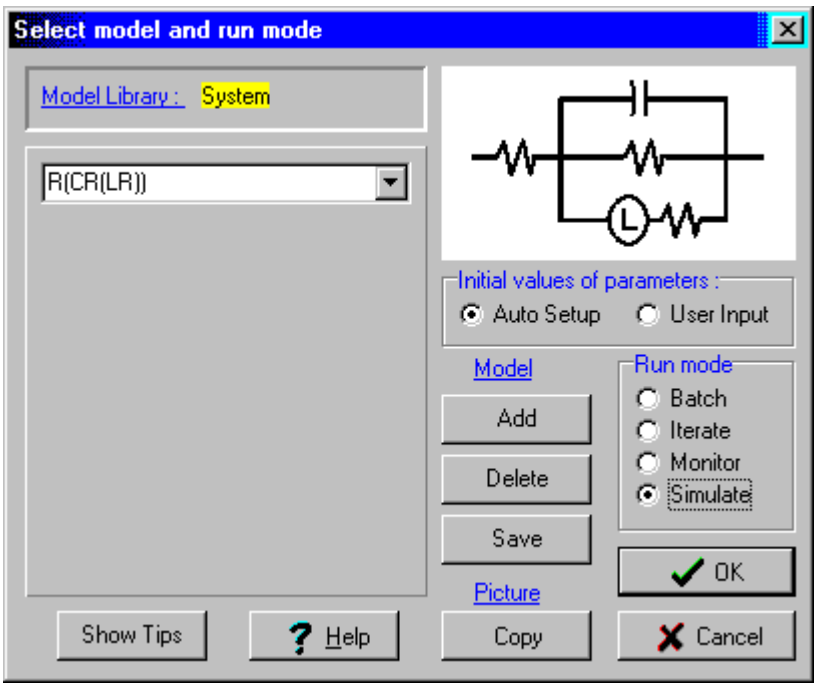
This feature is used to investigate the effects of parameters on plots.

Procedure

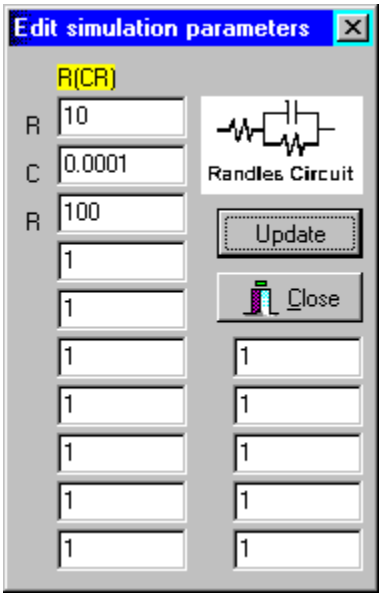
1. Click  . Click the drop-down button to expose the models in the drop-down list and choose **R(CR(LR))**.

2. Set Run mode to **Simulate**.

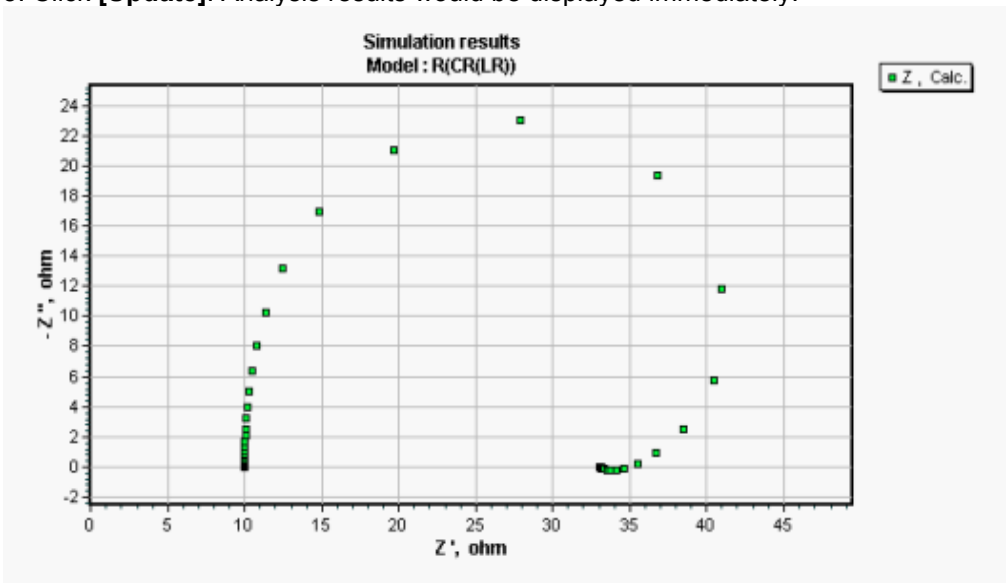
3. Click **[OK].**



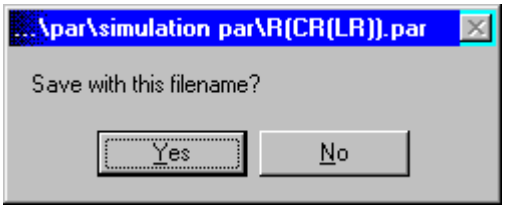
4. **Edit Simulation Parameters** dialog box appears on the top-right corner of the screen prompting input. Enter the values in the edit boxes associated with the parameters.



5. Click **[Update]**. Analysis results would be displayed immediately.



6. Click  . Save the results with the suggested name.



Try with other values of the parameters by following the Steps 4 and 5. (See Edit Simulation Parameters).

Next topic: Example 10

Example 10: Data for Dielectric Materials

For a dielectric material, dielectric constant is of interest. This property can be considered as capacitance. Can we use ZSimpWin to analyze data for dielectric materials?

Sample problem
Application Model **(HC)** to **...\data\HN Saved as Z Data.txt**?

Solution
Yes. ZsimpWin is capable of handling dielectric materials, and many models are already included in ZSimpWin, however, not documented at the present time. "H" represents "Havriliak-Negami" element. See S. Havriliak and S. Negami, J. of Polymer Science: Part C, No. 14, pp 99-117 (1966) for details.

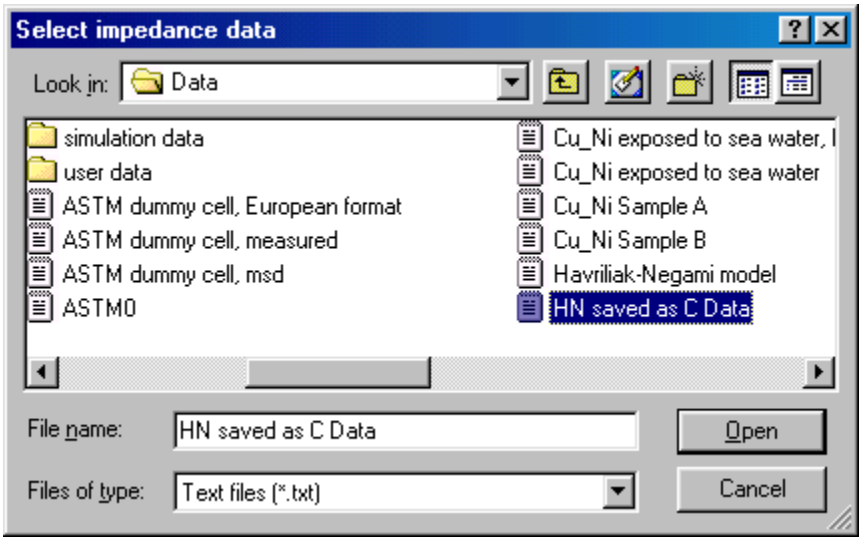
Equation : $Y(\omega) = j\omega(C_0 - C_\infty)\left[1+(j\omega\tau_0)^{\mu}\right]^{-\phi}$

Parameters : $(C_0 - C_\infty), \tau_0, \mu, \phi$

Procedure

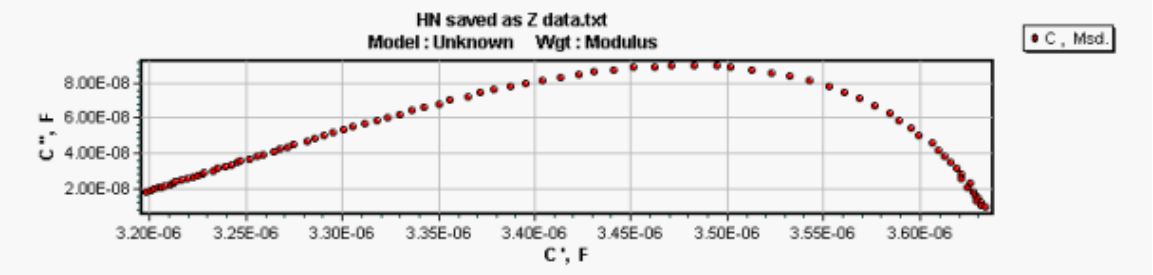
1. Click the **Dielectric System** on the **Dielectric** menu to activate the menus associated with dielectric materials. Now Bode, Admittance, and Real and Imag plots are associated with capacitance rather than impedance. Input data can be Impedance (frequency, Z', Z") or Capacitance (frequency, C', C"). The "File | Save Converted (C or Z Data)" Menu is provided to convert Z Data to C Data or C Data to Z Data.

2. Click  to display the **Select impedance data** dialog box. Select the file and click **[Open].**

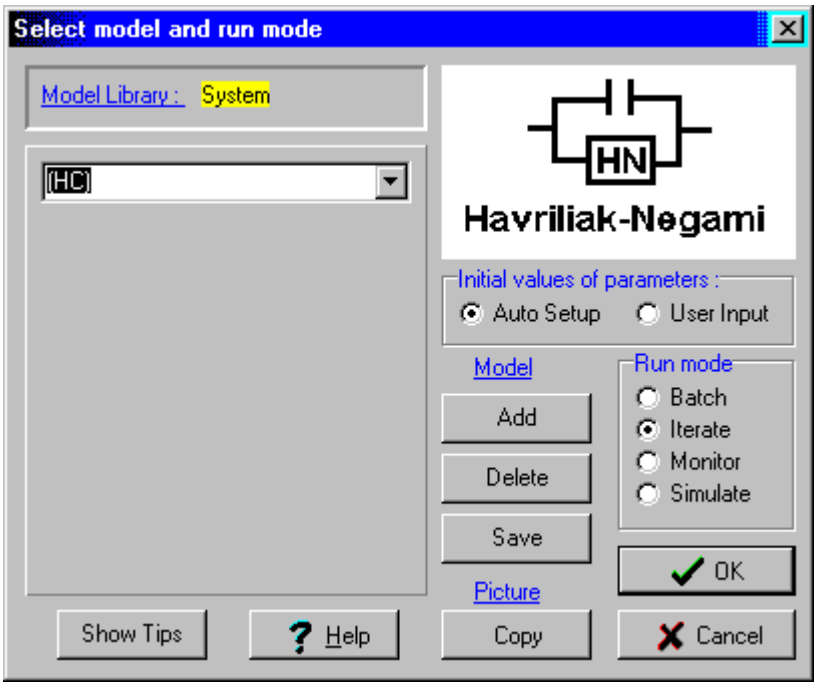


3. Click  to view the Capacitance plot

4 Uncheck the "**Fixed window**" checkbox to let ZSimpWin to adjust the window size to show all the data points in a rectangle which provides equal aspect ratio of the real and imaginary axes.



5. Click  .

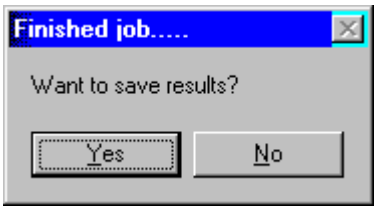


6. Click the drop-down button to expose the models in the drop-down list and choose **(HC)**. **Initial parameters** and **Run mode** options are set to **Auto Setup** and **Iterate** as default. If they have been changed from a previous run, reset these options.

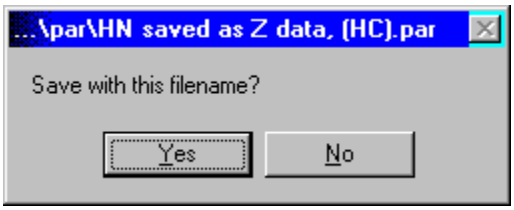
7. Click **[OK]**.

8. Wait until computation is finished. A small **Please wait...** dialog box will be shown on the top-left corner of the screen. This indicates the progress of computation.

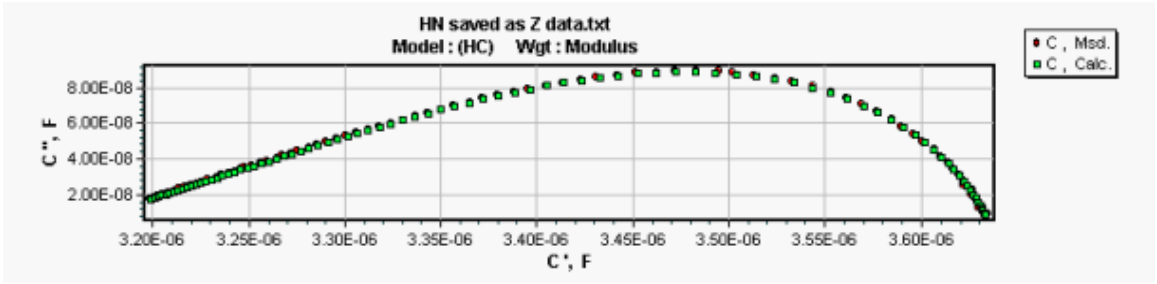
9. At the end of the computation, you are asked whether to save the results. Click **[Yes]**.



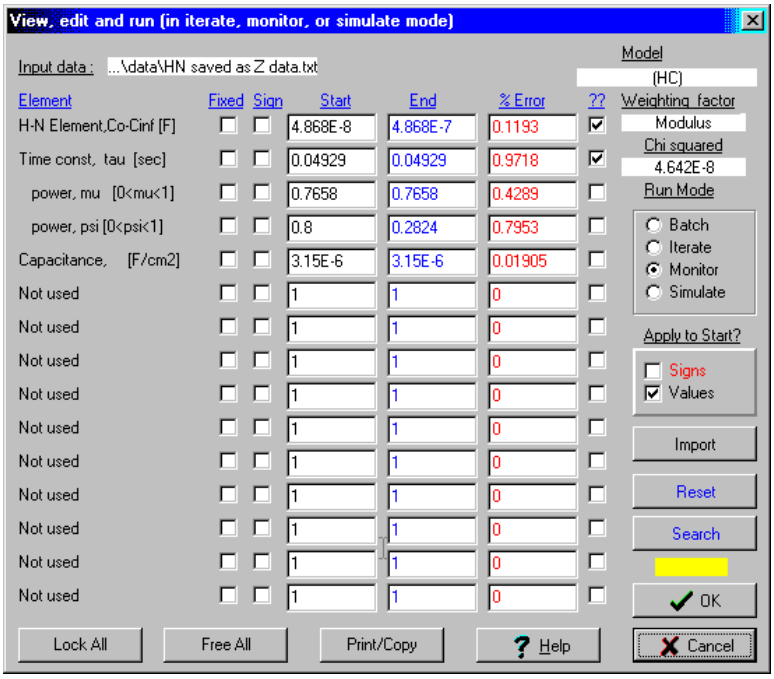
10. A save filename is suggested. Click **[Yes]**.



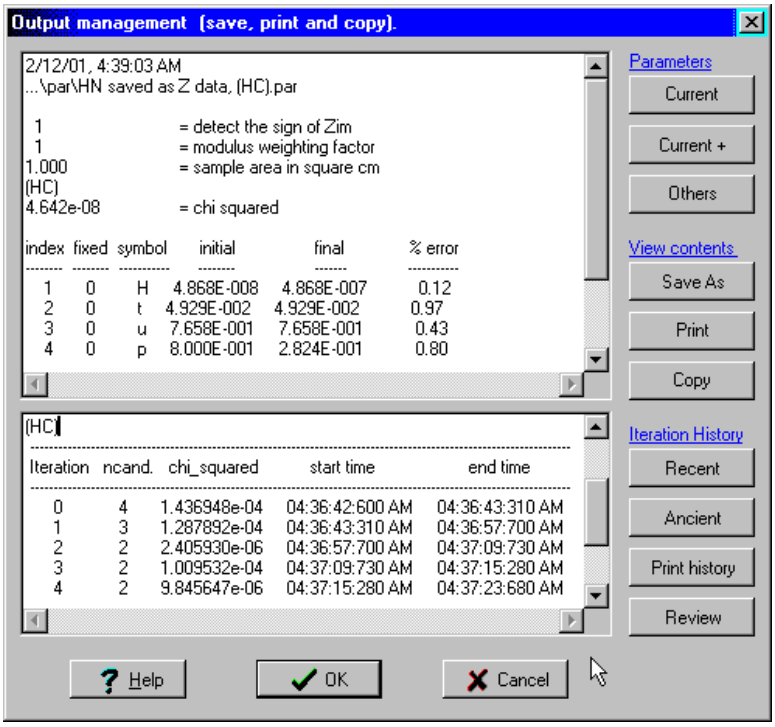
11. Examine the results for the Capacitance plot.



12. Examine the values of the estimated parameters.



13. Examine the parameters and iteration history.



Next topic: Input and Output

Input and Output

Available functions depend on

a) data types (text, plot),
b) input sources (File, Windows Clipboard), and
c) output targets (File, Screen, Printer, Windows Clipboard).

Input from File

Open File 

Retrieve Parameters 

Input from Windows Clipboard

Paste Z Data 

Output to File

Save parameters 
Save Impedance Data **File - Save Impedance Data**
Save Simulation Run **File - Save simulation**
Export Data **Tools - Export Data**

Save Plot 

Output to Screen and Printer
ZsimpWin follows the basic rule that the contents displayed on the screen can be printed.

(a) Iterate Mode and Simulate Mode

Estimated Parameters :  **[Current] [Print]**

Iteration History :  **[Recent] [Print History]**

Parameters and Plot :  **[Params + Current]**

Two plots :  **[2, Left, Portrait]**

Four plots :  **[4, All, Landscape]**

Multiple data sets in a plot 

Change of parameters with iteration :  **[Review] [Parameters] [Print]**

Change of chi-squared with iteration :  **[Review] [Chi-squared] [Print]**

(b) Batch Processing Mode

Batch Process Configuration :  **[Print]**

Check Progress :  **[Print]**

(**c) Extrapolation**
Extrapolation Results : **Extrapolate - [Find] [Print]**

(d) List of a Group
_Print File List in Project Group

Output to Windows Clipboard

Copy results (text) 

Copy displayed plot 

Copy the picture of selected model  **[Copy]**

Next topic: Estimated Parameters

Estimated Parameters

2/10/01, 8:09:32 AM
...\par\princetonAR par\Coating-3, R(Q(R(Q(R(Q(R(CR)))))).par

1	= detect the sign of Zim
1	= modulus weighting factor
1.000	= sample area
R(Q(R(Q(R(Q(R(CR)))))))	
1.948e-03	= chi squared

Index	fixed	symbol	Initial	final	% error
1	0	R	6.017E+000	6.059E+000	32.20
2	0	Q	1.325E-007	1.324E-007	5.52
3	0	N	8.917E-001	8.918E-001	0.60
4	0	R	2.825E+004	2.823E+004	2.92
5	0	Q	2.675E-006	2.676E-006	3.14
6	0	N	8.129E-001	8.126E-001	1.80
7	0	R	4.072E+005	4.075E+005	2.77
8	0	Q	5.776E-004	5.918E-004	60.30
9	0	N	8.000E-001	9.363E-001	12.40
10	0	R	3.748E+005	3.722E+005	22.70
11	0	C	5.648E-003	5.655E-003	14.70
12	0	R	9.947E+014	1.076E+015	1.01E11

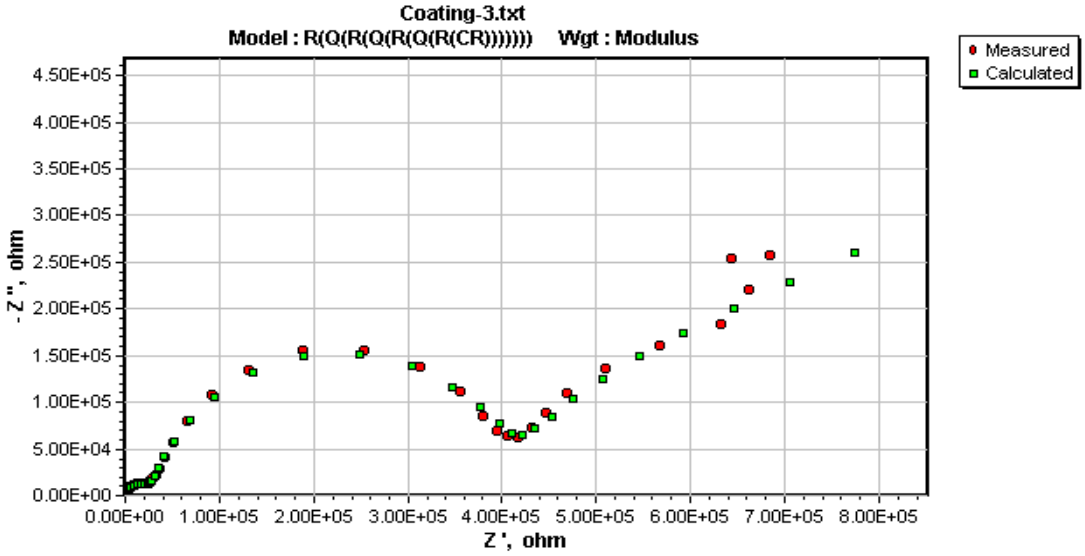
Parameters and Plot

Prints estimated parameters and displayed plot on a single page. The style of the displayed plot is selected by clicking on the "Nyquist", "Bode", "Re and Im", "Admittance", "Capacitance", and "Error" buttons.

2/10/01, 8:09:32 AM
...\par\princetonAR par\Coating-3, R(Q(R(Q(R(Q(R(CR)))))).par

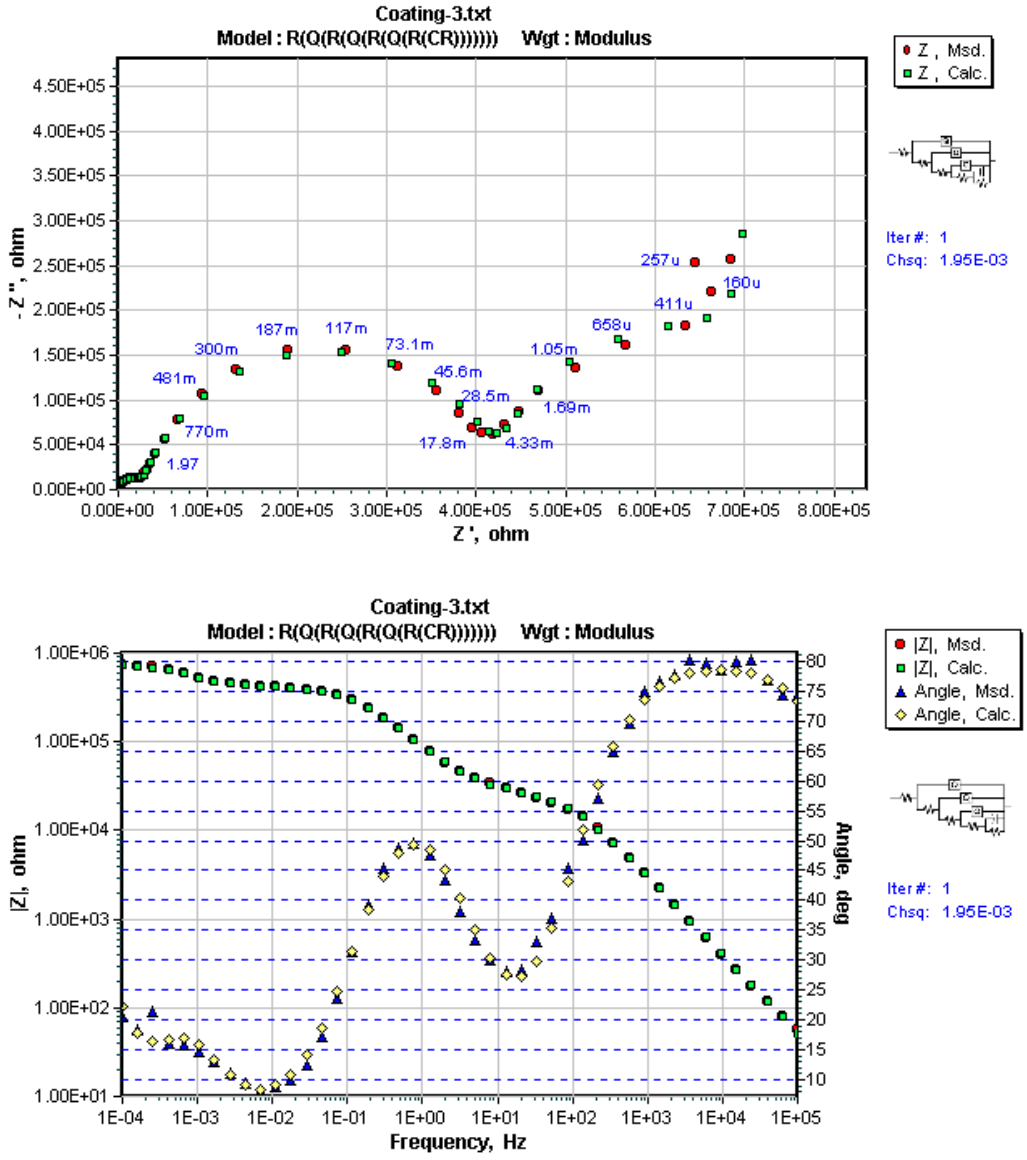
1	= detect the sign of Zim
1	= modulus weighting factor
1.000	= sample area
R(Q(R(Q(R(Q(R(CR)))))))	
1.948e-03	= chi squared

Index	fixed	symbol	Initial	final	% error
1	0	R	6.017E+000	6.059E+000	32.20
2	0	Q	1.325E-007	1.324E-007	5.52
3	0	N	8.917E-001	8.918E-001	0.60
4	0	R	2.825E+004	2.823E+004	2.92
5	0	Q	2.675E-006	2.676E-006	3.14
6	0	N	8.129E-001	8.126E-001	1.80
7	0	R	4.072E+005	4.075E+005	2.77
8	0	Q	5.776E-004	5.918E-004	60.30
9	0	N	8.000E-001	9.363E-001	12.40
10	0	R	3.748E+005	3.722E+005	22.70
11	0	C	5.648E-003	5.655E-003	14.70
12	0	R	9.947E+014	1.076E+015	1.01E11


Coating-3.txt
Model : R(Q(R(Q(R(Q(R(CR))))))) Wgt : Modulus
Measured
Calculated
-Z '', ohm
Z ', ohm
4.50E+05
4.00E+05
3.50E+05
3.00E+05
2.50E+05
2.00E+05
1.50E+05
1.00E+05
5.00E+04
0.00E+00
0.00E+00
1.00E+05
2.00E+05
3.00E+05
4.00E+05
5.00E+05
6.00E+05
7.00E+05
8.00E+05

Two Plots

Prints any of the first two plots selected in the **Print Item Selection** dialog box in a page. Prints in portrait orientation.



Next topic: Four Plots

Four Plots

Prints any of the first four plots selected in the Print Item Selection dialog box in a page. Prints in landscape orientation.

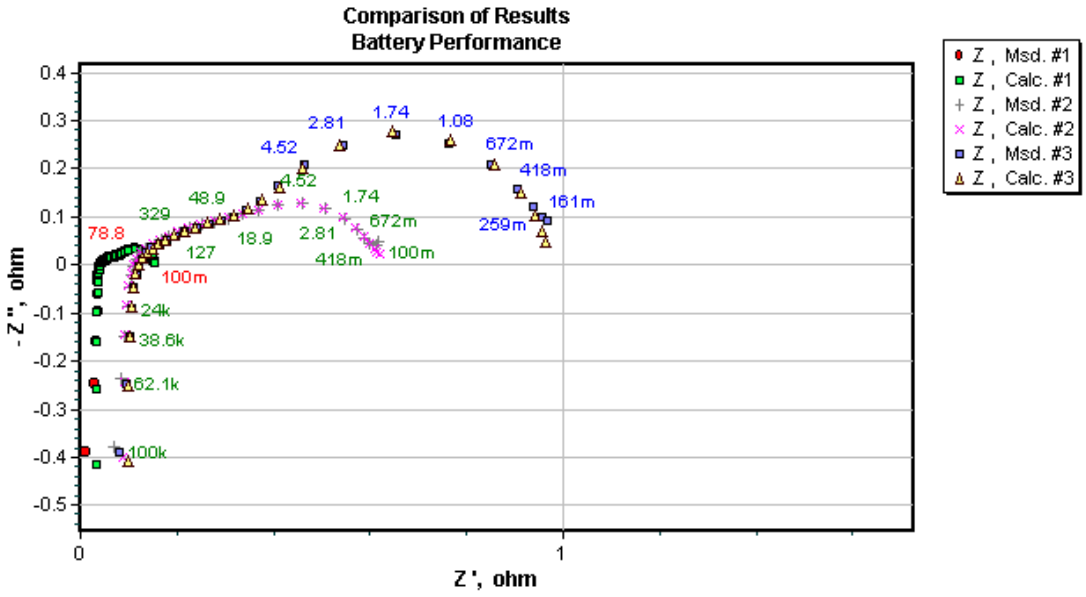
Next topic: Multiple data sets in a plot

Multiple data sets in a plot

See **Application Example E - Multiple data sets in a plot**.

12/31/01, 8:15:02 PM
C:\Program Files\ZSimpWin\report\Battery Performance.grp
C:\Program Files\ZSimpWin\data\princetonAR data\
C:\Program Files\ZSimpWin\par\princetonAR par\

3 = the number of files
Battery-2, LR(QR)(CR).par
Battery-3, LR(QR)(CR).par
Battery-4, LR(QR)(CR).par



Next topic: Iteration History

Iteration History

For each iteration, chi-squared value and the start and end times are saved as *.hst file.

2/10/01, 8:09:32 AM
...\hist\Coating-3, R(Q(R(Q(R(Q(R(CR)))))).hst
...\data\princetonAR data\Coating-3.txt
...\par\princetonAR par\Coating-3, R(Q(R(Q(R(Q(R(CR)))))).par

R(Q(R(Q(R(Q(R(CR)))))))

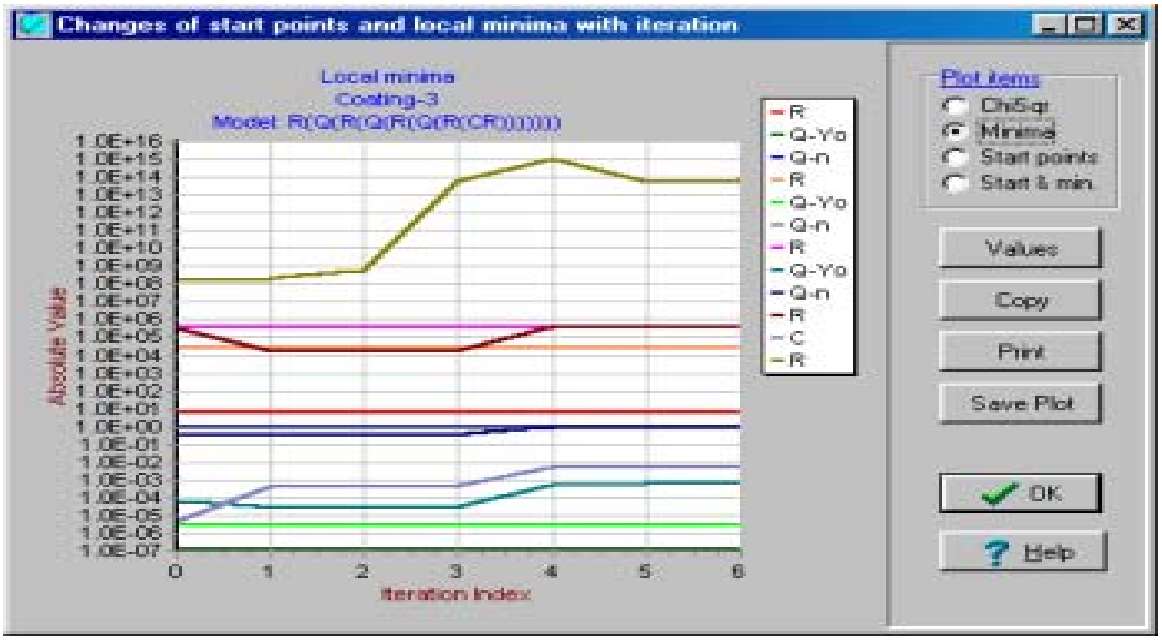
Iteration	# cand.	Chi_squared	start	end
0	4	3.195429e-03	05:50:49:260 PM	05:50:52:280 PM
1	2	2.473898e-03	05:50:52:280 PM	05:52:07:960 PM
2	4	2.473667e-03	05:52:07:960 PM	05:52:20:160 PM
3	4	2.473262e-03	05:52:20:160 PM	05:53:01:570 PM
4	2	1.955545e-03	05:53:01:570 PM	05:53:50:020 PM
5	2	1.947556e-03	05:53:50:020 PM	05:54:22:200 PM
6	2	1.948725e-03	05:54:22:200 PM	05:55:33:060 PM
7	2	1.947560e-03	05:55:33:060 PM	05:56:41:990 PM
8	2	1.947557e-03	05:56:41:990 PM	05:58:01:570 PM
9	2	1.947557e-03	05:58:01:570 PM	05:58:33:710 PM
10	2	1.947750e-03	05:58:33:710 PM	05:59:08:030 PM

Change of parameters with iteration

6/9/01, 12:21:33 AM
...\temp\Coating-3, R(Q(R(Q(R(Q(R(CR)))))).mat

R(Q(R(Q(R(Q(R(CR)))))))
6

symbol	0	1	2	3	4	5	6
R	5.819E+000	5.974E+000	5.986E+000	5.992E+000	6.105E+000	6.016E+000	6.019E+000
Q	1.344E-007	1.329E-007	1.329E-007	1.329E-007	1.329E-007	1.325E-007	1.325E-007
n	8.904E-001	8.914E-001	8.914E-001	8.915E-001	8.914E-001	8.917E-001	8.917E-001
R	2.876E+004	2.835E+004	2.834E+004	2.834E+004	2.831E+004	2.824E+004	2.824E+004
Q	2.552E-006	2.650E-006	2.651E-006	2.652E-006	2.668E-006	2.675E-006	2.675E-006
n	8.330E-001	8.170E-001	8.168E-001	8.167E-001	8.136E-001	8.129E-001	8.129E-001
R	3.685E+005	3.895E+005	3.908E+005	3.908E+005	4.049E+005	4.071E+005	4.071E+005
Q	5.852E-005	2.512E-005	2.510E-005	2.511E-005	4.959E-004	5.779E-004	5.780E-004
n	4.497E-001	3.358E-001	3.354E-001	3.354E-001	9.054E-001	9.318E-001	9.319E-001
R	2.984E+005	1.833E+004	1.613E+004	1.614E+004	3.874E+005	3.746E+005	3.746E+005
C	3.975E-006	4.088E-004	4.171E-004	4.171E-004	5.584E-003	5.648E-003	5.647E-003
R	1.769E+008	2.125E+008	5.156E+008	5.159E+013	1.111E+015	5.165E+013	6.062E+013
chisq	3.195E-003	2.474E-003	2.474E-003	2.473E-003	1.956E-003	1.948E-003	1.948E-003
ncand	4	2	4	4	2	2	2



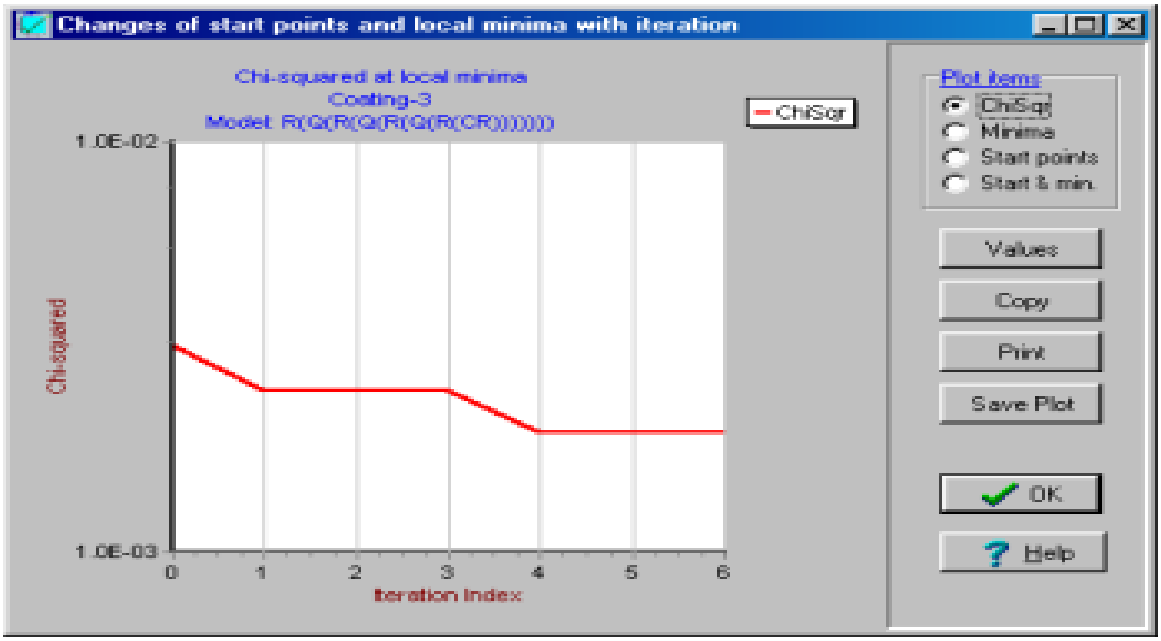
Next topic: Change of chi-squared with iteration

Change of chi-squared with iteration

6/9/01, 12:21:33 AM
...\temp\Coating-3, R(Q(R(Q(R(Q(R(CR)))))).mat

R(Q(R(Q(R(Q(R(CR)))))))
6

symbol	0	1	2	3	4	5	6
R	5.819E+000	5.974E+000	5.986E+000	5.992E+000	6.105E+000	6.016E+000	6.019E+000
Q	1.344E-007	1.329E-007	1.329E-007	1.329E-007	1.329E-007	1.325E-007	1.325E-007
n	8.904E-001	8.914E-001	8.914E-001	8.915E-001	8.914E-001	8.917E-001	8.917E-001
R	2.876E+004	2.835E+004	2.834E+004	2.834E+004	2.831E+004	2.824E+004	2.824E+004
Q	2.552E-006	2.650E-006	2.651E-006	2.652E-006	2.668E-006	2.675E-006	2.675E-006
n	8.330E-001	8.170E-001	8.168E-001	8.167E-001	8.136E-001	8.129E-001	8.129E-001
R	3.685E+005	3.895E+005	3.908E+005	3.908E+005	4.049E+005	4.071E+005	4.071E+005
Q	5.852E-005	2.512E-005	2.510E-005	2.511E-005	4.959E-004	5.779E-004	5.780E-004
n	4.497E-001	3.358E-001	3.354E-001	3.354E-001	9.054E-001	9.318E-001	9.319E-001
R	2.984E+005	1.833E+004	1.613E+004	1.614E+004	3.874E+005	3.746E+005	3.746E+005
C	3.975E-006	4.088E-004	4.171E-004	4.171E-004	5.584E-003	5.648E-003	5.647E-003
R	1.769E+008	2.125E+008	5.156E+008	5.159E+013	1.111E+015	5.165E+013	6.062E+013
chisq	3.195E-003	2.474E-003	2.474E-003	2.473E-003	1.956E-003	1.948E-003	1.948E-003
ncand	4	2	4	4	2	2	2



Next topic: Batch processing setup records

Batch processing setup records

1/14/02, 8:37:39 PM
C:\Program Files\ZSimpWin\batch\batch demo.cfg

1 = the number of models
R(CR)

...\data\princetonAR data\
...\par\princetonAR par\

4 = the number of files
Virgin coating-1.txt
Virgin coating-2.txt
Virgin coating-3.txt
Virgin coating-4.txt

Job identification
Virgin coating-1, R(CR).par : selected...
Virgin coating-2, R(CR).par : skipped...
Virgin coating-3, R(CR).par : selected...
Virgin coating-4, R(CR).par : selected...

Next topic: Batch processing run statistics

Batch processing run statistics

1/14/02, 8:30:32 PM
C:\Program Files\ZSimpWin\batch\batch demo.sta
C:\Program Files\ZSimpWin\data\princetonAR data\
C:\Program Files\ZSimpWin\par\princetonAR par\

4 = the number of available jobs

Virgin coating-1, R(CR).par
Completed.------ Start time, end time, and execution time :
1/14/02 8:30:28 PM
1/14/02 8:30:29 PM
00:01:150

Virgin coating-2, R(CR).par
Skipped...

Virgin coating-3, R(CR).par
Completed.------ Start time, end time, and execution time :
1/14/02 8:30:29 PM
1/14/02 8:30:31 PM
00:01:210

Virgin coating-4, R(CR).par
Completed.------ Start time, end time, and execution time :
1/14/02 8:30:31 PM
1/14/02 8:30:32 PM
00:01:100

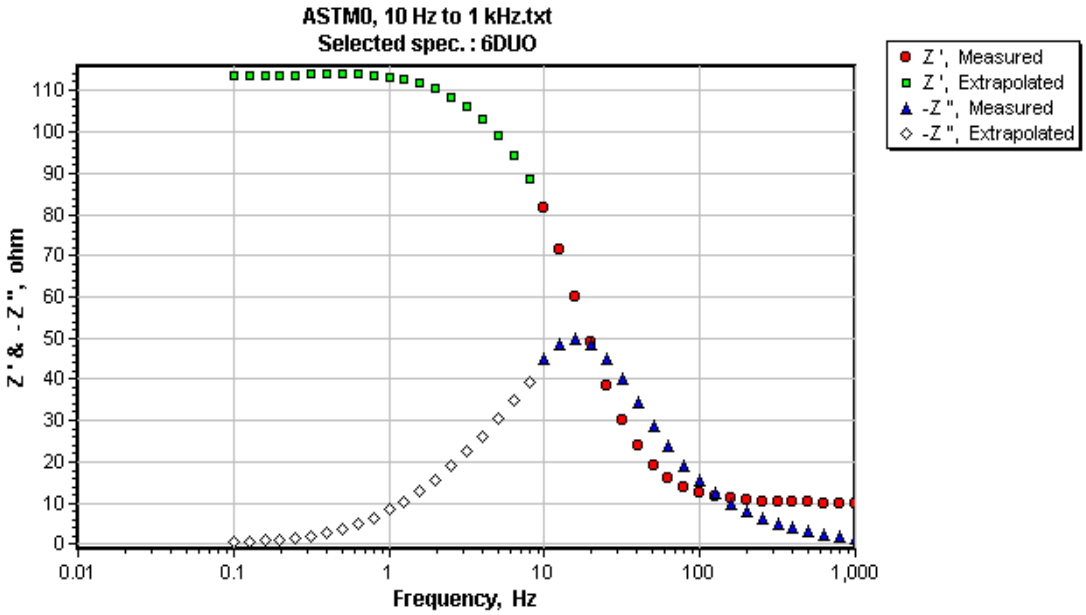
Next topic: Print Extrapolation Results

Print Extrapolation Results

4/18/01, 8:24:06 PM

...\temp\ASTM0, 10 Hz to 1 kHz.sum

order	Selection	Zr_inf+corr.	continuities	deviations	product
1	6DUO	1.090e+01	1.755e-02	1.838e-05	3.226e-07
2	7DUO	1.101e+01	1.283e-02	2.770e-05	3.554e-07
3	8DUO	1.100e+01	1.555e-02	2.379e-05	3.699e-07
4	5DUO	1.098e+01	1.417e-02	6.531e-05	9.256e-07
5	4DUO	1.063e+01	2.888e-02	7.033e-05	2.031e-06



Print File List in Project Group

3/22/01, 4:58:17 AM
C:\Program Files\ZSimpWin\report\test.grp
C:\Program Files\ZSimpWin\par\princetonAR par\

2 = the number of files
Battery-1, LR(Q(R(CR))).par
Battery-4, LR(Q(R(CR))).par

Next topic: Tools

Registration and technical support

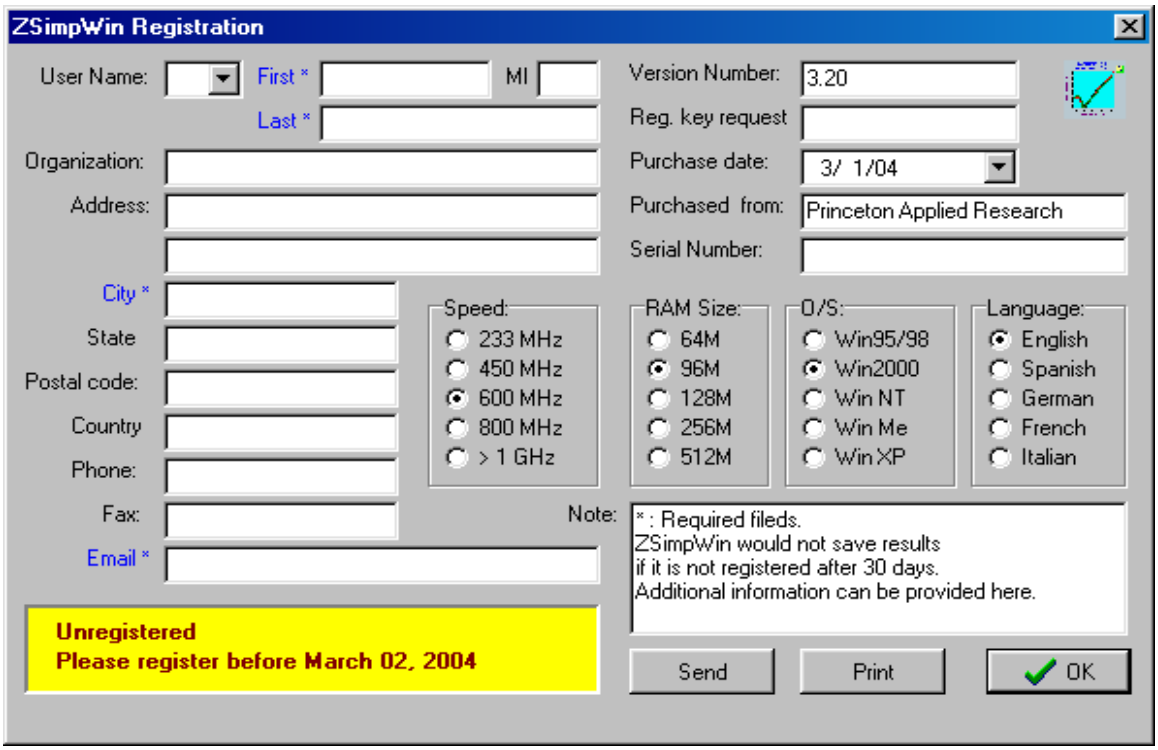
Instruction to register ZSimpWin and to request technical support.

Registration
Sending registration key request
Technical support

Next topic: Registration

Registration

ZSimpWin should be registered within 30-days of installation. If ZSimpWin were not registered, no results would be saved after data analysis. Click **Registration** on the **Help** menu. Fill out the registration form.



Do not type anything in the **Reg. key request** area. This name is assembled using the first two characters in your first name, the four characters in your last name, the two characters in the name of the city, and the file extension **".320"**. When the **[Send]**, **[Print]** or **[OK]** button is clicked, a **registration key request** is created in the Application folder. Send this file to Princeton Applied Research using one of the following methods:

1. Click on the **[Send]** button. Send the **registration key request** to: zsimpwin@pari-online.com as an email attachment (See Sending registration key request), or

2. Click on the **[Print]** button. Print the file and fax to: **(865) 425-1334**, or

3. Click on the **[Print]** button. Print the file and mail to:

Princeton Applied Research
801 South Illinois Ave.
Oak Ridge, TN 37830
ATTN: ZSIMPWIN REGISTRATION

A small **Registration key file** (????????.key) will be delivered to you via email. Make sure your email address is correct. When you receive this file, move it to the **Application folder** (**default = c:\Program Files\Zsimpwin**).

Sending registration key request

A **registration key request** (????????.320) has been created and then saved in your Application folder. The name of this file consists of the first two characters in your first name, the four characters in your last name, and the two characters in your city name.

Application folder = C:\Program Files \Zsimpwin (default)

1. Click zsimpwin@pari-online.com. You are ready to send a new email.

2. Type the subject as **Zsimpwin registration**.

3. Insert the **registration key request** (????????.320) as an email attachment.

4. Send this email.

Next topic: Technical support

Technical Support

With the purchase of the program, you have the right to get technical support. We would be happy to answer your questions. Send an email to:

zsimpwin@pari-online.com.

Please type the subject as **Technical support - Zsimpwin,** include your registration key request file name (????????.key), ZSimpWin version number, and operating condition (e.g., 850 MHz Pentium 4, 256 Mb, Windows 2000 Professional) in your email.

Feel free to visit the Princeton Applied Research site (www.princetonappliedresearch.com) or author's Web site (www.echemsw.com) to find information about product updates and technical notes.

Next topic: Acknowledgments

Acknowledgments

Princeton Applied Research accelerated the development of ZSimpWin by providing the following assistance to the author:

1. Princeton Applied Research performed alpha and beta tests and delivered reports to the author.
2. Princeton Applied Research allowed the author to use their impedance data to test the features in ZSimpWin. Some of these data are used to design Application Examples.
3. Mr. Bill Eggers expressed customers' needs of processing multiple data sets in sequence (batch processing) and presented his ideas about implementation.

The author cannot list numerous bug reports, critical comments, and suggestions provided by Princeton Applied Research's personnel.

Recently Dr. Derek Lenard (Dockyard Laboratory, Victoria, BC, Canada) advised the author to include sample area and data export features. He also allowed the author to use his data to design an Application Example.

Several trial users of old versions also provided insights to the development of ZSimpWin.

The author would like to express thanks to the professionals who provided exciting ideas, recommendations, and suggestions.

The author and Princeton Applied Research thoroughly tested the features in ZSimpWin. However it is possible that a software bug was not detected. Your bug reports and suggestions would be greatly appreciated for future enhancements.

February 2001

Bruno Yeum, Ph.D.
EChem Software
Ann Arbor, Michigan
USA