eistoolbox

for

Mathworks® MATLAB

A toolbox for batch fitting of Electrochemical Impedance Spectroscopy data to equivalent circuit models

User Guide

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Version 0.1-45

Contents

Chapter 1

Introduction

eistoolbox is a toolbox for MATLAB® used for batch fitting Electrochemical Impedance Spectroscopy (EIS) data to equivalent circuits.

Currently it is **alpha software**, and it will evolve over time.

1.1 Impedance Spectroscopy

Electrochemical Impedance Spectroscopy (EIS) measures the complex impedance of a sample as a function of the frequency. The experimental results are stored in two possible formats: polar coordinates (magnitude and phase) or rectangular coordinates (real and imaginary).

$$Z(f) = R + jX \tag{1.1}$$

where R is the resistance and X is the reactance of the sample.

The real part of the impedance is proportional to the resistivity, and the imaginary part is proportional to the permittivity. Both parameters can be calculated directly from the measurements, considering the exact geometry of the electrodes and measurement setup. For parallel plate electrodes, the following equations apply:

$$R = \frac{\rho L}{A} \tag{1.2}$$

$$C = \frac{\epsilon A}{D} \tag{1.3}$$

The capacitive reactance is given by

$$X_C = \frac{1}{2\pi f C} \tag{1.4}$$

Substituting (1.3) and (1.4) into (1.1) results in the following equation, which describes the impedance in terms of the resistivity and permittivity of the sample between parallel electrodes:

$$Z(f) = \frac{\rho L}{A} + \frac{1}{2\pi f}\frac{D}{\epsilon A} \tag{1.5}$$

Impedance Spectroscopy is also referred as Dielectric Spectroscopy, because it gives information about the dielectric properties of the measured sample.

1.2 Fitting to Equivalent Circuit Models

Experimental data is often fitted to equivalent circuit models. The models are designed to describe the interfaces, chemical processes and boundaries of the measured setup.

Chapter 2

Current capabilities of this software

It can accept any number of input files, both in CSV and Gamry DTA formats.

The CSV files should contain three columns with the impedance data, in the order: FREQ,REAL,IMAG.

The imaginary part can be positive or negative; the absolute value is taken inside the program before plotting.

The fitting algorithm uses the "fminsearch" function, implemented using the Zfit library from Jean-Luc Dellis.

It accepts any type of circuit model, built with serial and parallel elements, in the Zfit circuit string format.

The currently implemented elements are: resistors, capacitors, inductors and constant-phase elements (CPE).

The Warburg element can be implemented by using a CPE and setting the second parameter to 1/2.

2.1 Planned updates

In the future it will accept Levenberg-Marquard, Nelder-Mead, BFGS and Powell algorithms.

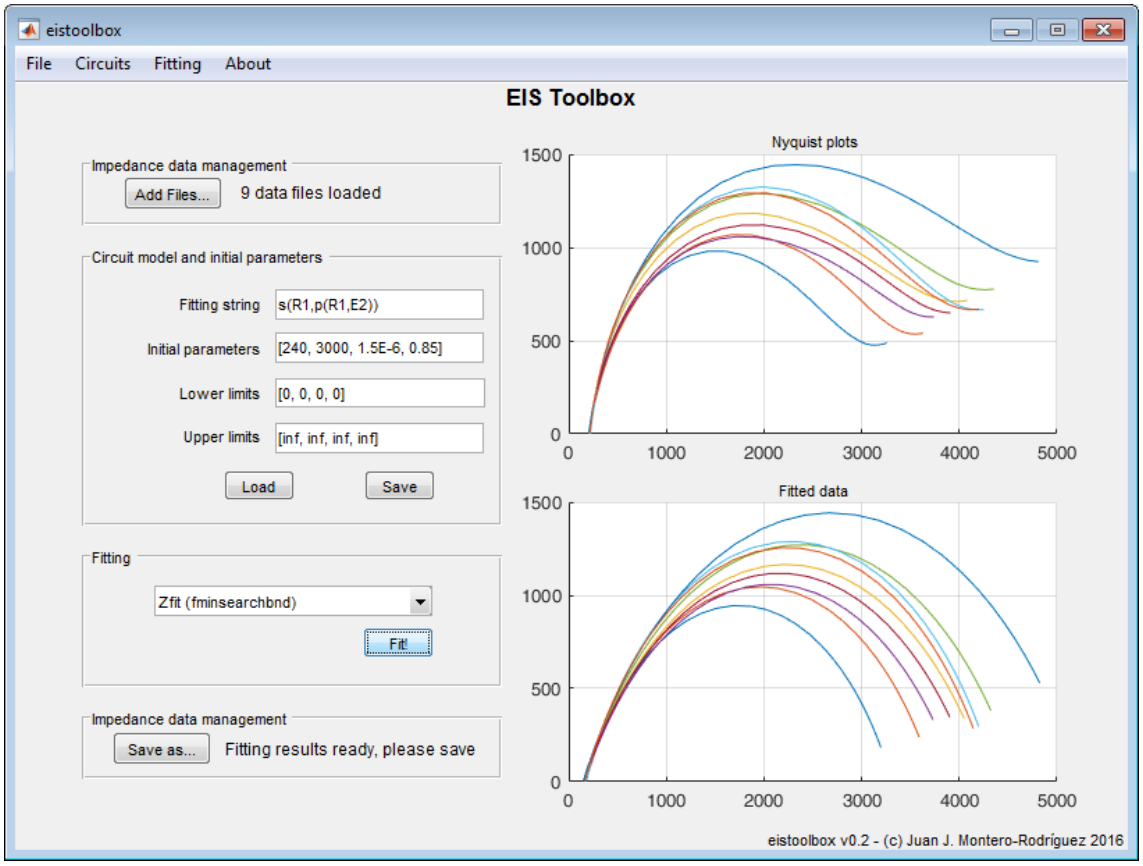
It will also include the error percentages of every fitting parameter, as well as the Pearson coefficient and correlation plot of the fitting results.

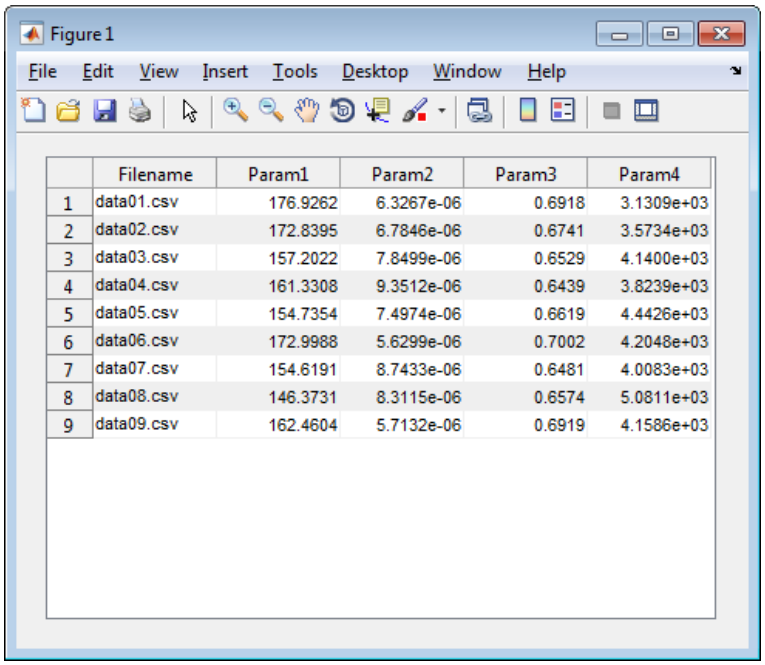
Chapter 3

Using the eistoolbox

3.1 Quick start guide

1. Add files using the "Add file..." button
2. Write the circuit string and fitting parameters (circuit string formatting)
3. Click the "Fit" button
4. Save the results using the "Save..." button





	Filename	Param1	Param2	Param3	Param4
1	data01.csv	176.9262	6.3267e-06	0.6918	3.1309e+03
2	data02.csv	172.8395	6.7846e-06	0.6741	3.5734e+03
3	data03.csv	157.2022	7.8499e-06	0.6529	4.1400e+03
4	data04.csv	161.3308	9.3512e-06	0.6439	3.8239e+03
5	data05.csv	154.7354	7.4974e-06	0.6619	4.4426e+03
6	data06.csv	172.9988	5.6299e-06	0.7002	4.2048e+03
7	data07.csv	154.6191	8.7433e-06	0.6481	4.0083e+03
8	data08.csv	146.3731	8.3115e-06	0.6574	5.0811e+03
9	data09.csv	162.4604	5.7132e-06	0.6919	4.1586e+03

Chapter 4

Algorithms

4.1 fminsearchbnd

Currently it supports only the fminsearchbnd function from Zfit.m

Chapter 5

Statistics

The program computes the following statistical parameters:

5.1 Linear regressions

Real of fitted vs Real of measured

Imag of fitted vs Imag of measured

MAG of fitted vs MAG of measured

5.2 Chi-square goodness of fit

$$\chi^2 = \sum_i^n \frac{(Observed_i - Expected_i)^2}{Expected_i}$$

Observed= fitted data

Expected= measured data

5.3 Error estimates for individual parameters

ToDo

Chapter 6

Licenses for included software

6.1 Zfit

The original file was released in 2005 and it is available here:

https://de.mathworks.com/matlabcentral/fileexchange/19460-zfit