UNIVERSITI PUTRA MALAYSIA

**DEVELOPMENT OF SOFTWARE FOR
DIELECTRIC ANALYSIS**

LIM LONG HSIANG

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DEVELOPMENT OF SOFTWARE FOR DIELECTRIC ANALYSIS

By

LIM LONG HSIANG

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for Degree of Master of Science

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Dedication

The author wishes to dedicate this paper to his family

his relative

his friends

his coursemates

for their love, support and encouragement

and

who made his years in the green campus beautiful and memorable

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment
of the requirements for the degree of Master of Science

DEVELOPMENT OF SOFWARE FOR
DIELECTRIC ANALYSIS

By

LIM LONG HSIANG

October 2002

Chairman : Zainul Abidin Hassan, Ph.D.

Faculty :   Science and Environment Studies

A software was developed using Visual Basic 6.0 for the study and analyzing of the
experimental data for the dielectric laboratory. For this purpose, a numerical
computation of Kramers-Kronig relations, fitting various dielectric functions and
plotting dielectric graphical representations were created and was found to achieve
high level of accuracy when compared with the simple non-interacting Debye model.
The software was used to analyze the experimental data of rose extract diluted in
water. The experimental data of rose extract diluted in water shows that the
polarisation consists of two different mechanisms, represented by a characteristic
loss peak and a strong low frequency dispersion. The mechanisms were in consistent
with the Kramers-Kronig relations and equivalent circuits were proposed for the
material under study.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai
memenuhi keperluan untuk ijazah Master Sains

PEMBANGUNAN PERISIAN UNTUK
ANALISIS DIELEKTRIK

Oleh

LIM LONG HSIANG

Oktober 2002

Pengerusi : Zainul Abidin Hassan, Ph.D.

Fakulti : Sains dan Pengajian Alam Sekitar

Sebuah perisian untuk tujuan mengkaji dan menganalisa data eksperimen untuk
makmal dielektrik telah dihasilkan dalam bahasa pengaturcara Visual Basic 6.0.
Untuk tujuan ini, satu perhitungan berangka hubungan Kramers-Kronig, penyesuian
fungsi-fungsi dielektrik dan pelakaran graf-graf dielektrik telah ditulis dan didapati
mencapai ketepatan yang tinggi apabila dibandingkan dengan model Debye yang
mudah dan tidak berinteraksi. Perisian ini digunakan untuk menganalisa data
eksperimen bagi ekstrak ros yang dicairkan dalam air. Data eksperimen untuk
ekstrak ros dicairkan dalam air menunjukkan bahawa pengkutuban terdiri daripada
dua mekanisme, iaitu puncak lesapan dan "dispersive" pada frekeunsi rendah.
Mekanisme-mekanisme ini adalah konsisten dengan hubungan Kramers-Kronig dan
litar-litar setara dicadangkan untuk sampel ini.

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Grateful thanks to my parent for their support and understanding.

I certify that an Examination Committee met on 4 October 2002 to conduct the final examination of Lim Long Hsiang on his Master of Science thesis entitled " Development of Software for Dielectric Analysis" in accordance with Universiti Pertanian Malaysia (Higher Degree) Act 1980 and Universiti Pertanian Malaysia (Higher Degree) Regulations 1981. The Committee recommends that the candidate be awarded the relevant degree. Members of the Examination Committee are as follows:

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The thesis submitted to the Senate of Universiti Putra Malaysia has been accepted as partial fulfillment of the requirements for the degree of Master of Science. The members of the Supervisory Committee are as follows.

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DECLARATION

I hereby declare that the thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at UPM or other instituitions.

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(signature)

LIM LONG HSIANG
Date: 13 / 11 / 2002

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LIST OF SYMBOLS

χ'	Real part of susceptibility
χ''	Imaginary part of susceptibility
ε'	Real part of permittivity
ε''	Imaginary part of permittivity
d	Distance between two parallel metallic electrodes (m)
ε_0	Permittivity of free space (Fm^{-1})
$\varepsilon(0)$	Static permittivity
P	Polarisation
V	Voltage (V)
Q	Charge (C)
E	Electric field (Vm^{-1})
R	Resistance (Ω)
C'	Real part of capacitance (F)
C''	Imaginary part of capacitance (F)
δ	Loss angle
ϕ	Phase angle between applied field
Y	Admittance (S)

CHAPTER 1

INTRODUCTION

1.1 General

The application of electrical insulation could be traced back to at least a century and a half. Scientists and engineers had begun to show interest in the dielectric properties as early as 1870s and since then systematic and extensive investigations have been made on the properties of dielectric materials. It is known that engineers and technologists searching for the insulating materials were more concerned with the specific applications of the material than fundamental physical mechanism governing the behavior of these materials. By contrast with the insulation aspect, the study of dielectric phenomena are more concerned with the microscopic mechanism governing the dielectric polarisation especially the transient behavior under the time-varying electrical fields. One of the most important concepts to be developed concerned the induced and orientational polarisation was that by Clausius and Mossotti in the 1870s. This treatment concerned the static response represents the earliest attempt to approach the many- body system (Jonscher, 1983). The other concept was the one developed by Debye on the treatment of the dynamic dielectric response of freely floating dipoles, such as might be found in dipolar liquid. This opened up a new era in the investigations of the frequency and time-dependence of the dielectric response.

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1.2 An Introduction to the Dielectric Response

The dielectric response of many materials have always been studied for a long time. With the availability of advanced and modern measuring equipment, a great wealth of experimental data are available for interpretation. However, difficulties in obtaining the precise physical characteristic of these materials from the experimental data was one of the biggest problem concern.

One aspect of the dielectric reponse is the apparent "universality" of the form of the dielectric response which has been known for the quarters of a century under the name of the Curie-Von-Scweider Law (Jonscher, 1983). This law states that the discharge or de-polarisation currents of a wide range of the dielectric materials follow the power law of time dependence. The unrivalled range of the dynamic variables of time and frequency of the experimental data is further enhanced by the principle of time-temperature or frequency-temperature superposition which enable the data taken at different temperatures to be related to one another, thereby increasing the range and reliability of these data.

The length of the dynamical range shows the entire time and frequency range, from frequencies corresponding to nuclear energies of 10 G eV, down to the reciprocal age of the Universe – a total of 40 decades. The inertia, phonon and quantum processes dominates the behavior at frequency in over THz.

At the most basic level it is possible to differentiate between the static response and the dynamic response to time-varying electrical fields. One particular aspect of time-dependent behavior relates to the decay of polarisation from an initial stage to zero after the sudden removal of an initial field. This decay is known as dielectric relaxation in the case of "low" frequency range and it can be shown that it is linked to the dielectric response under the sinusoidal varying electric fields.

1.3 Charge Carrier

All matter consists of positive and negative charges at the atomic scale, where these charges balance each other at microscopic as well as macroscopic level: the former corresponding to overall charge neutrality, the latter giving rise to local space charge. For example, in the case of metals, the valence electrons constitute a cloud of negative charges which is neutralised by the fixed positive charge of atomic core.

In a neutral molecule, a local charge imbalance caused by the distorted charge distribution creating a dipole, in which the separation of the charges may be fixed or may be related to the magnitude of the locally prevailing electric field. For the case of the separation charge that is fixed, it is caused by chemical interactions between *dissimilar* atoms forming the molecule, for example HCl. For the case of HCl, the different electron affinities of the each atom contribute to the appearance of the net charges on each atom and thus creating a permanent dipole. For the case of the separation related to the magnitude of the locally prevailing field, it is result of chemical interactions and the separation occurs between the outer valence electrons

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and the atomic cores.

1.4 Objectives

This project involved the development of software capable to

1) carry out Kramers-Kronig transformation for the measured data.

2) plot different graphical representations for dielectric properties.

The purpose of plotting different graphical representations such as complex admittance, impedance and permittivity is to determine the equivalent circuit of the sample and the mechanism involved.

CHAPTER 2

LITERATURE REVIEWS

2.1 Kramers-Kronig Relations

The Kramers-Kromig relations was first derived by Kronig in 1926 and Kramers in 1927 (Frohlich, 1958). They are applicable to all dissipative systems and are the consequences of the principle of casuality.

Lovell (1974) has developed a program for numerical computation of the Kramers-Kronig transformations in BASIC. This program transforms the directly measured data of the real part of capacitance into the corresponding frequency related conductance. The program extrapolates the measured data by one decade at either end.

Lee (2001) also develops a program for Kramers-Kronig transformation in Visual Basic 5.0. In his work, he had used the Debye equation to check the accuracy of the computation and was found to have good agreement with the equation except at the range of less than 3 decades below the peak frequency.

2.2 Dielectric Spectra

The relation between the complex susceptibilty or permittivity and the frequency was first established by Debye (Jonscher, 1983). This relation was known as *Debye Dispersion equation* and was applicable for gases and dilute solutions by assuming that the free molecules did not interact with each other. However, the behavior of most of dielectric materials departs greatly from the model suggested by Debye. This lead to a modification proposed by Cole and Cole with small departure from the ideal Debye model (Jonscher, 1983). Davidson and Cole proposed another formula. Navrilliak and Negami has combined the Cole-Cole and Cole-Davidson expressions and has been capable of fitting many of the observed results (Jonscher, 1983). Another formula was proposed by Jonscher (1983). Hill (1978) has discovered a generalised empirical relationship for the loss curve that includes the Cole-Cole and Cole-Davidson functions as particular cases and was in good agreement with the experiment.

Shin and Yeung (1989) derive an alternative loss equation. This loss formula is derived from consideration of the Jonscher formula (Jonscher, 1983) and its parameters were chosen so that it is possible to obtain a close expression for real susceptibility by explicit integration of the Kramers-Kronig relations. It proved to be useful in fitting experimental data.

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CHAPTER 3

THEORY

3.1 Electric Susceptibility and Permittivity

Consider a capacitor of value C_0 in vacuum .It is then filled with a dielectric material, it's capacitance increases to a value of C. There is a change in capacitance ΔC. The ratio of the increase of the capacitance ΔC to capacitance in vacuum C_0

$$\chi' = \frac{\Delta C}{C_0} = \frac{C - C_0}{C_0} = \frac{C}{C_0} - 1 \qquad (3.1)$$

where χ' is the *electrical susceptibility.*

The electrical permittivity, ε' is defined as the ratio of the capacitance C of a capacitor filled with a dielectric to the value C_0 of the same capacitor under vacuum, i.e

$$\varepsilon' = \frac{C}{C_0} \qquad (3.2)$$

From equation (3.1) and (3.2), we get relation between susceptibilty and permittivity as

$$\chi' = \varepsilon' - 1 \qquad (3.3)$$

The electric susceptibility and permittivity are defined as non-dimensional.

If current flows through the capacitor which is in phase with applied field then it will contribute to the energy loss of conductivity in the material which fills the capacitor. For

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that reason, it is more convenient to express the electric susceptibility and permittivity as complex numbers as complex numbers provides phase angle of the component of polarisation.

Consider a dielectric in an A.C circuit. If a capacitor of capacitance C_0 under the voltage V is filled with a dielectric, its capacitance increases by ΔC, and consequently, the charge on the plates increases by Δq. The relation is given by

$$\Delta C = \frac{\Delta q}{V} \tag{3.4}$$

Assuming the alternating voltage of angular frequency ω is sinusoidal, i.e

$$V = V_0 e^{i\omega t} \tag{3.5}$$

The change in the strength of the current Δi flowing in the capacitor circuit as a result of introduction of a dielectric is given by

$$\Delta i = \frac{d(\Delta q)}{dt} = \Delta C \frac{dV}{dt} = i\omega \Delta C V = \Delta i_0 \exp\left[i(\omega t + \frac{\pi}{2})\right] \tag{3.6}$$

where $\Delta i_0 = \omega \Delta C V_0$ and $i = e^{j\pi/2}$.

From equation (3.6), we know that the current in the capacitor circuit out of phase the voltage by 90^0. This was the case of loss-free capacitor.

In a capacitor filled with a lossy dielectric, a current which is separated by the discharge current, flows in phase with the applied field and was given by

$$i_s = \frac{V}{R} \tag{3.7}$$

Therefore, the resultant change in the current density is given by

$$\Delta I = \Delta i + i_s = (i\omega\Delta C + \frac{1}{R})V \tag{3.8}$$

The phase difference ϕ between the applied field and change in the intensity Δi is less than 90^0. The dielectric loss is represented by resistance, R. The phase angle of a dielectric is, from equation (3.7) and (3.8)

$$\tan\phi = \frac{i_s}{\Delta i} = \frac{1}{\omega R\Delta C} \tag{3.9}$$

A lossy dielectric can be described using the notation of complex susceptibility χ in the form of

$$\chi = \chi' - i\chi'' \tag{3.10}$$

where χ' is the real part of susceptibility, χ'' is the imaginary part of susceptibility and i $= \sqrt{-1}$.

The change in the intensity of the current ΔI flowing in the capacitor circuit given by the dielectric is given by

$$\Delta I = i\omega\chi C_0 V = (i\chi' + \chi'')\omega C_0 V \tag{3.11}$$

The tangent of loss angle is given by

$$\tan\delta = \frac{\varepsilon''}{\varepsilon'} \tag{3.12}$$

where ε' is the real part of permittivity and ε'' is imaginary part of permittivity. The tangent of the loss angle is frequently used as a measure of dielectric loss. The electrical conductivity of a dielectric is given by

$$\sigma = \omega\chi'' \tag{3.13}$$

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The complex susceptibility describes the macroscopic properties of a dielectric in electric fields at different frequencies. Similarly, the tangent of the loss angle can also be given by

$$\tan \delta = \frac{\chi''}{\chi'+1} \qquad (3.14)$$

The behavior of a dielectric in an electrical field is described by the polarisation vector which relates the intensity of the polarising field to the electrical susceptibility while the permittivity relates the displacement vector and the field intensity vector.

3.2 Dielectric Polarisation

The relative shift of the positive and negative charges in matter is referred to as dielectric polarisation. The relationship between the polarisation P and field E is given by:

$$P = \varepsilon_0 \chi E + \text{ higher term} \qquad (3.15)$$

The first term proportional to the field E is of dominant importance in most system, ε_0 is the permittivity of the free space and χ is the susceptibility. The polarisation P is directly related to the surface charge which appears on a polarised medium. A planar capacitor consisting of two parallel metallic electrodes at a distance, d apart. And let the space to be empty initially. If the voltage V is applied between the electrodes, this gives rise to the uniform field E =V/d, and charges $\pm Q_0 = \pm\varepsilon$ E appear on the plates as a consequences of the Gauss Law. Now let the space between the electrodes be filled

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with a medium of susceptibility χ which becomes polarised in its own right, contributing a surface charge $Q_1 = P$, so that the total charge on the electrodes becomes the sum of the contribution of free space and the contribution due to the material medium polarisation:

$$Q = Q_0 + Q_1 = \varepsilon_0 (1 + \chi)E = \varepsilon(0)E \qquad (3.16)$$

This equation defines the static permittivity $\varepsilon(0)$ of the material, in terms of the contributions of the free space and of the material.

3.3 Polarisation of Static Electric Fields

Polarisation arises from a finite displacement of charges in a steady electric field. Permanent and induced type dipole are polarising species which are incapable of leading to a continuing conduction current in a static electric field because the charges cannot be separated under normal conditions. The dissociation of dipole can only be achieved if the field is sufficiently strong enough to break the bonding forces of the dipolar molecules in the solid.

Generally, there are two types of polarisation, induced and oriented. Induced polarisation is caused by the deformation of the charge distribution. Induced deformation includes electronic and atomic polarisation. Orientation polarisation results from the directional effect of the field on the permanent dipole moments of molecules.