

ANALYSIS OF HEAT FLOW IN RESISTIVE SWITCHING DEVICES USING BOUNDARY INTEGRAL EQUATION



M.Sc THESIS

BY

GEZAHEGN KASAYE

A THESIS SUBMITTED TO
THE PROGRAM OF APPLIED MATHEMATICS
SCHOOL OF APPLIED NATURAL SCIENCE

IN PARTIAL FULFILLMENT OF THE REQUIREMENT FOR THE DEGREE OF
MASTER'S OF SCIENCE IN APPLIED MATHEMATICS

OFFICE OF GRADUATE STUDIES
ADAMA SCIENCE AND TECHNOLOGY UNIVERSITY

ADAMA, ETHIOPIA
January 2, 2018

Analysis of Heat flow in Resistive Switching Devices using Boundary Integral Equation



M.Sc Thesis

By
Gezahegn Kasaye

Advisor
Tamirat Temesgen (Ph.D)

A Thesis Submitted to the Program of Applied Mathematics
School of Applied Natural Science

Presented in Partial Fulfillment of the Requirement for the Degree of Master's of Science in Applied
Mathematics

©Copyright Adama Science and Technology University

Adama, Ethiopia
January 2, 2018

ADAMA SCIENCE AND TECHNOLOGY UNIVERSITY

Author: Gezahegn Kasaye

Title: Analysis of Heat flow in Resistive Switching Devices using Boundary Integral Equation

Program: Applied Mathematics

Degree: M.Sc. Convocation: July Year: 2016

Authors Signature

ADAMA SCIENCE AND TECHNOLOGY UNIVERSITY
APPLIED MATHEMATICS PROGRAM

I hereby certify that I have read and evaluated this thesis titled “Analysis of Heat flow in Resistive Switching Devices using Boundary Integral Equation” prepared under my guidance by Gezahegn Kasaye. I recommend that it be submitted as fulfilling the thesis requirement.

Tamirat Temesgen(Ph.D)

Advisor

Signature

Date

As member of the board of Examiners of the M.Sc Thesis Open Defense Examination, we certify that we have read and evaluated the thesis entitled “Analysis of Heat flow in Resistive Switching Devices using Boundary Integral Equation” prepared by Gezahegn kasaye and examined the candidate. We recommend that the thesis be accepted as fulfilling the thesis requirement for the degree of Master of Science in Mathematics (Defferential).

Examining Committee

Gezahegn Kasaye

Student

Signature

Date

Tamirat Temesgen(Ph.D)

Advisor

Signature

Date

Chair person

Signature

Date

Internal Examiner

Signature

Date

External Examiner

Signature

Date

Dep't.Head

Signature

Date

Sch.Dean

Signature

Date

Sch. Grad. Studies Dean

Signature

Date



Abbreviation and Notation

Ω	A simply connected bounded region in $\mathbb{R}^3$.
Γ	The boundary of Ω .
$C^0(\Gamma)$	A set of all continuous functions on Γ (or boundary).
$C^1(\Gamma)$	A set of all continuous functions and differentiable on Γ .
$C^2(\Omega)$	The set of all continuous functions and twice differentiable on Ω .
$C(\Omega)$	The space of continuous functions in Ω .
$\nabla \cdot \vec{F}$	Divergence of the function $\vec{F}$
∇	The gradient operator.
Δ	Laplace's operator.
δ	Diracs delata function.
$\mathbb{R}$	The set of real numbers.
BIE	Boundary Integral Equation.
$\frac{\partial u}{\partial n}$	The partial derivative of the function u with respect to the unit outward normal.

Declaration

By my signature below, I declare that this thesis is my own work. I have followed all ethical and technical principles of scholarship in the preparation, and compilation of this thesis. Any scholarly matter that is included in the thesis has been given recognition through citation. This thesis is submitted in partial fulfillment of the requirements for a Differential calculus degree at Adama science and Technology University. The thesis is deposited in the Adama science and Technology University Library and is made available to borrowers under the rules of the Library. I solemnly declare that this thesis has not been submitted to any other institution anywhere for the award of any academic degree, diploma or certificate. Brief quotations from this thesis may be made without special permission provided that accurate and complete acknowledgement of the source is made. Requests for permission for extended quotations from or reproduction of this thesis in whole or in part may be granted by the Head of the School or department when in his or her judgment the proper use of the material is in the interest of scholarship. In all other instances, however, permission must be obtained from the author of the thesis.

Name: Gezahegn Kasaye Gebre

Date _____

Department: Mathematics

Signature _____

Acknowledgement

First of all, thanks to God, for giving me endurance and patience in accomplishing this piece of work. Any accomplishment requires the effort of many people and this work is not different. I would like to extend my great thanks to my advisor, **Dr. Tamirat Temesgen** for his great continuous support, encouragements, helpful comments, advice and interesting discussions on the subject of this paper through out the academic year. In fact, words can not express my heartfelt gratitude, appreciation and thanks for all the support, guidance and time he had provided during my thesis work (especially his great unforgettable contribution in introducing me with the $\text{\LaTeX}$). At the last but not the least, my special thanks are due my sister Alem kasaye the provision of the necessary support to complete the postgraduate study at Adama science and Technology University. Likewise, I wish to thank all the authors whose works played an important role in the success of this thesis work.

Abstract

In this thesis, we analyze the Boundary Integral Equation(BIE) methods for the poisson equation with Dirichlet Boundary Conditions in three dimensions where the boundary is smooth. We present a formulation of solving the BIEs reformulated from the poisson boundary value problems. BIE is particularly attractive in developing integral equation methods, it reduces the dimensions of the problem and often transforms a problem in an infinite domain to integrals on the finite boundary. A Boundary value problem for Partial Differential Equation with a constant coefficient can be reduced to a BIE by using the fundamental solution and Greens representation formula, we reduced the boundary value problem into Boundary Integral Equations. Boundary integral equation Method is developed for the problem of heat conduction in a geometry composed of an insulator between two metallic electrodes, with multiple cuboidal heat sources within the insulator.

Table of Contents

Dedication	i
Abreviation and Notation	ii
Declaretion	iii
Acknowledgement	iv
Abstract	v
Table of Contents	vi
List of Figures	viii
1 Introduction and Background	1
1.1 Statement of the problem	3
1.2 Objectives	4
1.2.1 General objectives	4
1.2.2 Specific objectives	4
1.3 Significant of the study	4
2 Literature review	5
3 Mathematical Preliminaries	7

3.1	Partial Differential Equations (PDE's)	7
3.1.1	Elliptic PDE's ($b^2 - 4ac < 0$) [steady-state in time]	8
3.2	Boundary value problem	8
3.2.1	Boundary Conditions for Elliptic PDE's:	9
3.3	Integral equation	9
3.4	Greens identities	12
3.5	BIE method for poisson equation with Dirichlet boundary condition	14
3.5.1	Fundamental solution	15
4	Analysis of Heat flow in Resistive Switching Devices	20
4.1	Problem Formulation	20
4.2	Formulation of Boundary Integral Equation for the Resistive Switching Devices . . .	21
5	Conclusion	26
	References	27

List of Figures

1.1	Schematic diagram of a typical resistive switching device.	1
1.2	Schematic profile view of device, with two filaments (represented by two cuboidal heat sources) close to each other. The top and bottom electrodes have thermal conductivities k_1 and k_3 , whereas the insulator has a thermal conductivity of k_2	3
3.1	A three dimensional physical domain	14
4.1	The Composite device in space	20
4.2	Top electrod	21
4.3	Insulator	22
4.4	Botom electrod	23

Chapter 1

Introduction and Background

Resistive switching refers to the physical phenomena where a dielectric suddenly changes its (two terminal) resistance under the action of a strong electric field or current. The change of resistance is non-volatile and reversible. Typical resistive switching systems are capacitor like devices, where the electrode is an ordinary metal and the dielectric a transition metal oxide. The electrode may be Au, Pt, Al, Ag, $SrRuO_3$, etc. the dielectric TMO(transition metal oxide) may be TiO_2 , HfO_2 , NiO, $SrTiO_3$, PCMO, LSMO, YBCO, etc[1].

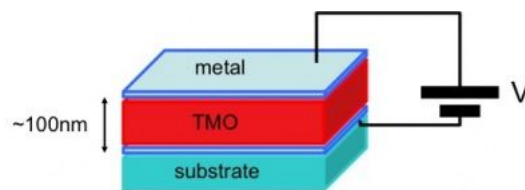


Figure 1.1: Schematic diagram of a typical resistive switching device.

The effect of sudden and non-volatile change of the resistance due to the application of electric stress, typically voltage or current pulsing, may allow the fabrication of future novel electronic memory concepts, such as non-volatile random access memories (RAM), hence, it is also termed resistive RAM, RRAM, or ReRAM. While non-volatile memory effects have been reported in a huge variety of systems, here we shall be concerned with those based on Transition Metal Oxides (TMO). In fact, TMOs in typical systems Fig.(1.1) usually exhibit high dielectric constants, which is considered a desirable feature towards dense electronic integration. Resistive random-access memory (RRAM or ReRAM) is a type of non-volatile (NV) random-access (RAM) computer memory that works by changing the resistance across a dielectric solid-state material often referred to as a memristor[1].

An **Electrode** is an electrical conductor used to make contact with a nonmetallic part of a circuit (e.g. a semiconductor, an electrolyte, a vacuum or air). The word was coined by William Whewell at the request of the scientist Michael Faraday from the Greek words elektron, meaning amber (from which the word electricity is derived). Electrodes are used to provide current through nonmetal objects to alter them in numerous ways and to measure conductivity for numerous purposes. Examples

include: Electrodes for fuel cells, Electrodes for medical purposes, such as for recording brain activity, recording heart beats, electrical brain stimulation, recording and delivering cardiac stimulation, Electrodes for electrophysiology techniques in biomedical research, Electrodes for execution by the electric chair, Electrodes for electroplating, Electrodes for arc welding, Electrodes for cathodic protection, Electrodes for grounding, and Electrodes for chemical analysis using electrochemical methods etc[2].

An **Insulator** is a material whose internal electric charges do not flow freely; very little electric current will flow through it under the influence of an electric field. This contrasts with other materials, semiconductors and conductors, which conduct electric current more easily. The property that distinguishes an insulator is its resistivity; insulators have higher resistivity than semiconductors or conductors. A perfect insulator does not exist, because even insulators contain small numbers of mobile charges (charge carriers) which can carry current[2].

Thermal conductivity (often denoted by k) is the property of a material to conduct heat. It is evaluated primarily in terms of Fourier's Law for heat conduction. Heat transfer occurs at a lower rate across materials of low thermal conductivity than across materials of high thermal conductivity. Correspondingly, materials of high thermal conductivity are widely used in heat sink applications and materials of low thermal conductivity are used as thermal insulation. The thermal conductivity of a material may depend on temperature. The reciprocal of thermal conductivity is called thermal resistivity. Thermal conductivity is actually a tensor, which means it is possible to have different values in different directions[3].

Many problems of physics are formulated as second-order PDEs e.g. wave equation, diffusion (heat) equation, Helmholtz equation, Schrodinger equations. These PDEs can describe a wide variety of phenomena such as sound, heat. From this we can study about a problem solving for Steady state heat equation in resistive switching device. We will take a Greens second identity(Representation formula) by using explicit knowledge of a fundamental solution of the differential equation, BVPs can be reduced to BIEs. However, the fundamental solution is only available for linear PDEs with constant coefficients.

In this thesis, we present a direct method formulation for solving the boundary integral equation reformulated from the poisson BVP. The integral equation method is an elegant mathematical way of transforming elliptic PDE into BIE. The BIE Method is a powerful tool for solving certain BVPs. It is particularly attractive in developing integral equation methods. Since, when applied, it reduces the dimensions of the problem and often transforms a problem in an infinite domain to integrals on the finite boundary. A BVP for PDE with a constant coefficient can be reduced to a BIE [4].

There are two distinct methods for reducing constant coefficients BVP to a BIEM: direct and indirect ones. The construction of these two types is based on different approaches. The former start from the representation formula, where the solution at any point in the domain is expressed in terms of its boundary value and its image under the associated boundary operator. If the problem models a physical situation, then the unknown functions have a direct physical significance, see e.g., [5]. The first integral formulation is often derived through the application of the second Greens identity, while the second integral formulation is founded on single or double layer potentials. It is from the assumption that the solution can be expressed in terms of a source density function defined on the

problems boundary. The method of BIEs has always had two important applications in the theory of BVPs for PDEs: as a theoretical tool for proving the existence of solutions and as a practical tool for the construction of solutions [6]. Both methods yield a single integral equation for a single unknown function.

BIEs are the most important tool for BVPs in PDEs. Many BVPs of mathematical physics and engineering can be reduced to integral equations over the boundary of the domain of interest. According to the BIE method, the BVP is replaced by an integral equation posed on the boundary (or on a portion of it) of the considered domain. The key tool in applying the BIE method is the construction of an appropriate fundamental solution of the problem, which satisfies some of the BCs (e.g., Dirichlet Boundary Condition). Then, by applying Greens theorem we sought solution. Finally, we obtain an integral representation of solution [7].

Any mathematical model of switching device [8]-[15], must include the heat equation,

$$\nabla \cdot (k \nabla T) = -Q,$$

where k is the thermal conductivity and Q is the power density. The thermal timescales are typically much shorter (on the order of picoseconds) than the timescales associated with ionic conduction [8]; the device may therefore be assumed always to be in the thermal steady state, thus obviating the need to include the heat capacity term in the heat equation. Efficient thermal modeling is advantageous in rapidly scanning the parameter space of these devices for device optimization.

1.1 Statement of the problem

Consider a three-layered device of lateral dimensions l_x and l_y . Let the metal electrodes have thicknesses of t_1 and t_3 and the insulator h . The device is illustrated schematically in the profile view in Figure 1.2,

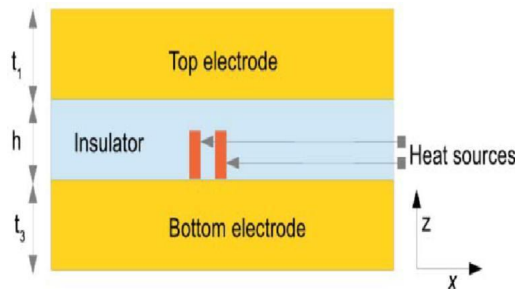


Figure 1.2: Schematic profile view of device, with two filaments (represented by two cuboidal heat sources) close to each other. The top and bottom electrodes have thermal conductivities k_1 and k_3 , whereas the insulator has a thermal conductivity of k_2 .

Let $T_i(x, y, z)$, $i = 1, 2, 3$ be the temperature profile in the two electrodes and in the insulator with k_i , $i = 1, 2, 3$ are corresponding thermal conductivity. The heat equation there reads

$$\nabla \cdot (k_i \nabla T_i) = -S_i(x, y, z). \quad (1.1)$$

where $S_i(x, y, z)$, $i = 1, 2, 3$ arbitrary source of power-density profile in the electrodes and insulator. We assume that there is no heat source in the two electrodes, i.e., $S_1 = S_3 = 0$.

Using boundary integral equation method, we will solve the heat equation in the three layers independently, and combine the solutions together such that both continuity of the temperature and continuity of the heat-flux are satisfied across the two boundaries between the two electrodes and the insulator. Therefore, in this study we try to address the following basic question

- How we formulate Boundary integral equation for each layer of composite device?
- What is the solution of heat equation in a metal-insulator-metal structure?

1.2 Objectives

1.2.1 General objectives

The main objective of this study is to analyze the heat flow in a metal-insulator-metal structure using boundary integral equation method.

1.2.2 Specific objectives

The specific objective of the study are:

- i. To formulate Boundary integral equation to heat equation in each layer of a metal-insulator-metal structure by applying Green's second identity.
- ii. To determine the solutions of heat equation in a metal-insulator-metal structure by BIEM.

1.3 Significant of the study

The significance of the study is to

- i. Understand the mechanism of heat flow through resistive switching device.
- ii. Understand the application of Green's second identity.

Chapter 2

Literature review

Partial differential equations (PDEs) have numerous essential applications in various fields of science and engineering such as electromagnetic theory, elasticity, fluid mechanics, thermodynamic, heat transfer, Physics etc. In the mid eighteenth century, physical problems such as the conduction patterns of heat and the study of vibrations and oscillations led to the study of Boundary integral equation[47].

In past several decades many authors mainly had paid attention to study the solution of steady state partial differential equations by using various developed method such as Boundary integral equation method(BIEM), Fourier series method, Finite element method (FEM), Finite difference method (FDM), Continued Fraction Method and Sine-Cosine method. Recently, researchers have applied the Boundary integral equation Method successfully to obtain analytic solution.

For example: The boundary integral equation method is used to study Stress intensity factors for semi-elliptical surface cracks in pressurised cylinders[16]. The boundary integral equation method used for treatment of singularities in the calculation of stress intensity factors[17]. The boundary integral equation method used for plate flexure with conditions inside the domain[18]. The boundary integral equation method used to analyze clamped plates on elastic foundation[19].

The boundary integral equation method used for the study of Stress analysis of pressure vessels and piping[20]. The boundary integral equation method used for radiation and scattering of elastic waves in three dimensions[21]. The boundary integral equation methods used to study eigenvalue problems of elastodynamics and thin plates[22]. The boundary integral equation method used to study the solution of problems involving elastic slabs[23].

The boundary integral equation method used to study a quadratic formulation for two-dimensional elastoplastic analysis[24]. The boundary integral equation method used for Analysis of mixed mode fracture and crack closure[25]. The boundary integral equation method used for three-dimensional analysis of electromagnetic fields in rectangular waveguides[26]. The boundary integral equation method used for three-dimensional design optimization[27]. The boundary integral equation method used for optimum shape design and positioning of features[28]. The boundary integral equation

method used for analysis of three dimensional transient acoustic wave propagation[29].

The boundary integral equation method used to study the steady state Oscillation problems for anisotropic bodies[30]. The boundary integral equation method used for numerical study of elastic wave scattering by cracks or inclusions[31]. The boundary integral equation method used to study Stress singularities for three-dimensional corners[32]. The boundary integral equation method used to solve embedded planar crack problems under shear loading[33]. The boundary integral equation method used in the prediction of dielectric characteristics of humidified composite insulator glass/epoxy core[34]. In 2005 C. Y. Dong, Kang Yong Lee used the boundary integral equation method for Numerical analysis of doubly periodic array of cracks/rigid-line inclusions in an infinite isotropic medium[35].

The boundary integral equation method and boundary element methods to Degenerate scale for the analysis of circular thin plate[36]. The boundary integral equation method used for Permeance computation[37]. The boundary integral equation method for the solution of a class of problems in anisotropic elasticity[38]. The boundary integral equation method used to path planning for autonomous mobile robots[39]. The boundary integral equation method used to study the frequency domain for cracks under transient loading[40].

The fractional integral transform and a finite cosine Fourier integral transform used to solve Analytical solution for the 3D steady state conduction in a solid subjected to a moving rectangular heat source and surface cooling[41]. Reproducing kernel particle method (RKPM) used to obtain numerical solution of three-dimensional steady-state heat conduction problems[42]. variable separation method used to obtain Analytical Solutions of Three Dimensional Steady-State Heat Transfer in Rectangular Ribs[43]. Variable separation method and superposition method used to obtain Analytical solutions of the steady or unsteady heat conduction equation in industrial devices: A comparison with FEM results[44].

Therefore, this study is aimed to develop a scheme to find the analytic solution of steady state heat conduction in composite device by Boundary integral equation method. The gap observed is the researcher used the Boundary integral equation method as new method to obtain analytical solution, which is not likely (presumably) present in the existing literature. The significance of this study is eventually, it may be expected that the present special issue would certainly help to explore the researchers with their new arising problems. Because at the present, the use of partial differential equations and integral equations are commonly encountered in the fields of science and engineering. This issue has addressed some efficient computational tools, recent trends, and developments regarding the analytical and numerical methods for the solutions of partial differential equations and integral equations arising in physical models.

Chapter 3

Mathematical Preliminaries

3.1 Partial Differential Equations (PDE's)

A PDE is an equation which includes derivatives of an unknown function with respect to two or more independent variables. PDE's describe the behavior of many engineering phenomena such as: Wave propagation, Fluid flow (air or liquid), Vibration, Mechanics of solids, Heat flow and distribution, Electric fields and potentials, Diffusion of chemicals in air or water, Electromagnetism and quantum mechanics.

Definition 3.1 (PDE, [46]) let $u = u(x_1, \dots, x_n)$ be a function of n independent variables $x_1, \dots, x_n$. A PDE is an equation that contains the independent variables $x_1, \dots, x_n$, the dependent variables or the unknown function u and its partial derivatives up to some order. It has the form:

$$F(x_1, \dots, x_n, u, u_{x_1}, \dots, u_{x_n}, u_{x_1x_1}, \dots, u_{x_ix_j}, \dots) = 0$$

where, F is a given function and $u_{x_j} = \frac{\partial u}{\partial x_j}$, $u_{x_ix_j} = \frac{\partial^2 u}{\partial x_i \partial x_j}$, $i, j = 1, \dots, n$ are the partial derivatives of u .

Definition 3.2 (Linear first order PDE, [46]). A Linear first order PDE in two independent variables x, y and the dependent variable u has the form:

$$a(x, y)u_x + b(x, y)u_y + c(x, y)u = d(x, y) \quad (3.1)$$

where, $a, b, c, d \in C^1(\Omega)$, $\Omega \subset \mathbb{R}^2$ and $a^2 + b^2 \neq 0$. If we consider the differential operator

$$L := a \frac{\partial}{\partial x} + b \frac{\partial}{\partial y} + c$$

then equation 3.1 can be written as $LU = d$; while the homogeneous equation corresponding to (3.1) is $LU = 0$.

Definition 3.3 (Linear second order PDE, [46]). A linear second order PDE in two independent variables x, y is given by:

$$a(x, y)u_{xx} + b(x, y)u_{xy} + c(x, y)u_{yy} + d(x, y)u_x + e(x, y)u_y + f(x, y)u = g(x, y) \quad (3.2)$$

where, $a, b, c, d, e, f, g \in C^2(\Omega)$, $\Omega \subseteq \mathbb{R}^2$ and $a^2 + b^2 + c^2 > 0$ in Ω . If we consider the partial differential operator

$$L\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right) := a \frac{\partial^2}{\partial x^2} + b \frac{\partial^2}{\partial x \partial y} + c \frac{\partial^2}{\partial y^2} + d \frac{\partial}{\partial x} + e \frac{\partial}{\partial y} + f,$$

then (3.2) is written as $LU = g$; while the homogeneous equation corresponding to (3.2) is $LU = 0$.

Classification of PDE From equation (3.2)

If $b^2 - 4ac < 0$ Elliptic PDE (e.g. Laplace Eq.)

If $b^2 - 4ac = 0$ Parabolic PDE (e.g. Heat Eq.)

If $b^2 - 4ac > 0$ Hyperbolic PDE. (e.g. Wave Eq.)

Each category describes different phenomena.

3.1.1 Elliptic PDE's ($b^2 - 4ac < 0$) [steady-state in time]

- Typically characterize steady-state systems (no time derivative)
temperature, torsion, pressure, membrane displacement and electrical potential.
 - closed domain with boundary conditions expressed in terms of $u(x, y)$, $\frac{\partial u}{\partial n}$ (in terms of $\frac{\partial u}{\partial x}$ and $\frac{\partial u}{\partial y}$).
- Typical examples include**

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \begin{cases} 0 & \text{Laplace Eq.} \\ -D(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}) & \text{Poisson Eq.} \end{cases}$$

Where $a = 1, b = 0, c = 1 \Rightarrow b^2 - 4ac = -4 < 0$

3.2 Boundary value problem

In the field of differential equations, a boundary value problem is a differential equation together with a set of additional constraints, called the boundary conditions. A solution to a boundary value problem is a solution to the differential equation which also satisfies the boundary conditions.

Definition 3.4 (Boundary value problem, [45]) is a problem, typically an ordinary differential equation or a partial differential equation, which has values assigned on the physical boundary of the domain in which the problem is specified.

3.2.1 Boundary Conditions for Elliptic PDE's:

Dirichlet: u provided along all of edge

Neumann: $\frac{\partial u}{\partial n}$ provided along all of the edge (derivative in normal direction)

Definition 3.5 *Dirichlet boundary condition [45] (the first kind) specifies the values of the solution itself (as opposed to its derivative) on the boundary, Examples For ordinary differential equation for instance,*

$$y'' + y = 0$$

the dirichlet boundary condition on the interval $[a,b]$ take the form

$$y(a) = \alpha, \quad y(b) = \beta,$$

where α and β are given numbers. For partial differential equation

$$\nabla^2 y + y = 0$$

where ∇^2 denote the Laplace operator. the dirichlet boundary conditions on the domain $\Omega \subset \mathbb{R}^n$ take the form

$$y(x) = f(x) \quad \forall x \in \partial\Omega$$

where f is known function defined on the boundary $\partial\Omega$.

Definition 3.6 *Neumann boundary condition[45] In mathematics, the Neumann (or second-type) boundary condition is a type of boundary condition, named after Carl Neumann. When imposed on an ordinary or a partial differential equation, the condition specifies the values in which the derivative of a solution is applied within the boundary of the domain. For partial differential equation for instance*

$$\nabla^2 y + y = 0$$

where ∇^2 denote the Laplace operator. the Neumann boundary conditions on the domain $\Omega \subset \mathbb{R}^n$ take the form

$$\frac{\partial y}{\partial n}(x) = f(x) \quad \forall x \in \partial\Omega$$

where n denotes (typically exterior) normal to the boundary $\partial\Omega$ and f is given scalar function. The normal derivative which shows up on the left side is defined as

$$\frac{\partial y}{\partial n}(x) = \nabla y(x) \cdot n(x)$$

where ∇ is the gradient(vector) and the dot is the inner product.

3.3 Integral equation

Recall that a differential equation is an equation containing an unknown function under a differential operator. Hence, we have the same for an integral equation.

An integral equation in which an unknown function appears under an integral sign [51].

Definition 3.7 *Fredholm integral equation of first type is given by*

$$f(x) = \int_a^b K(x,t)\psi(t)dt$$

where ψ is unknown function, f is known function, K is another known function of two variables often called the kernel function.

Definition 3.8 *Fredholm integral equation of second type is given by*

$$\psi(x) = f(x) + \lambda \int_a^b K(x,t)\psi(t)dt$$

where, where the kernel $K(x,t)$ and forcing (or inhomogeneous) term $f(x)$ are known functions and $\psi(x)$ is the unknown function. Also, the parameter λ ($\in \mathbb{R}$ or $\mathbb{C}$) is unknown factor.

Definition 3.9 *Volterra integral equations of the first and second kind take the forms*

a)

$$f(x) = \int_a^x K(x,t)\psi(t)dt$$

b)

$$\psi(x) = f(x) + \lambda \int_a^x K(x,t)\psi(t)dt$$

respectively

Note: Volterra equations may be considered a special case of Fredholm equations. Suppose $a \leq t \leq b$ and put

$$K(x,t) = \begin{cases} K(x,t) & \text{for } a \leq t \leq x, \\ 0 & \text{for } x \leq t \leq b, \end{cases}$$

then

$$\int_a^b K(x,t)\psi(t)dt = \left(\int_a^x + \int_a^b \right) K(x,t)\psi(t)dt = \int_a^x K(x,t)\psi(t)dt + 0.$$

Test Functions

In order to compute the locally averaged values of a distribution, the notion of a test function is required. A function $v(x)$ defined on an open set $\Omega \subset \mathbb{R}^3$ is said to have compact support if $v(x) = 0$ for x in the complement of a compact subset of Ω . In particular, if $\Omega = \mathbb{R}^3$, then v has compact support if there is a positive constant, C such that $v(x) = 0$ for $|x| > C$. We say that $v(x)$ is a test function if v has compact support and, in addition, v is infinitely differentiable on Ω [49].

Definition 3.10 (Test Functions) Let Ω be a domain in $\mathbb{R}^3$. Then, the set

$$D(\Omega) = \{v \in C^\infty(\Omega) : \text{supp}(v) \text{ is compact in } \Omega\}$$

is called the set of test function. The set $D(\Omega)$ is also denoted by, $C_0^\infty(\Omega)$.

For instance, the function given by

$$v(x, y, z) = \begin{cases} e^{\frac{1}{(x^2+y^2+z^2)-1}}, & \text{if } x^2 + y^2 + z^2 < 1 \\ 0 & \text{otherwise} \end{cases}$$

is a test function in $\mathbb{R}^3$. The support of v is closed unit ball, i.e., $\text{Supp } v = \{(x, y, z) : x^2 + y^2 + z^2 \leq 1\}$ and it is infinitely differentiable function.

Note that, if $v_1(x), v_2(x), v_3(x)$ are test functions on Ω , so is $C_1v_1 + C_2v_2 + C_3v_3$ for any $C_1, C_2, C_3 \in \mathbb{R}$. The space $D(\Omega)$ is therefore a real linear space.

Definition 3.11 (Locally integrable)

i) Let Ω be open set in $\mathbb{R}^3$ and a function $u : \Omega \rightarrow \mathbb{C}$ is said to be locally integrable if

$$\int_K |u| dx < \infty \text{ for all compact subset } K \text{ of } \Omega.$$

Any continuous function is locally integrable.

ii) A locally integrable function defines a distribution in the following:

$$\text{if } v \in D(\Omega), \text{ then } u(v) := \langle u, v \rangle = \int_{\Omega} u v dx$$

Distribution

A generalizations of the classical concept of functions which used to formulate solutions of partial differential equations is known as Distributions. A distribution is a linear functional on a space of test functions [49].

Definition 3.12 (Distribution) Let Ω be a domain in $\mathbb{R}^3$ and $D(\Omega)$ be the space of test function. The set of distributions (or generalized functions) denoted by $D'(\Omega)$ is the collection of all complex-valued

linear continuous functionals u over $D(\Omega)$, i.e.,

$$u : D(\Omega) \rightarrow \mathbb{C}$$

where the value of u acting on v denoted by

$$u(v) := uv := \langle u, v \rangle$$

satisfies the following linearity and continuity criteria

For any $\alpha, \beta, \gamma \in \mathbb{C}$ and $v_1, v_2, v_3 \in D(\Omega)$

1. $\langle u, \alpha v_1 + \beta v_2 + \gamma v_3 \rangle = \alpha \langle u, v_1 \rangle + \beta \langle u, v_2 \rangle + \gamma \langle u, v_3 \rangle$,
2. $\langle u, v_n \rangle \rightarrow \langle u, v \rangle$ for $n \rightarrow \infty$ in $\mathbb{C}$, whenever $v_n \rightarrow v$ in $D(\Omega)$.

Dirac delta function

Mathematically, the Dirac delta function is defined by how it behaves inside an integral in fact the first operation where Dirac used the delta function is the integration in distribution sense [48]:

Definition 3.13 The symbol $\delta(x)$ is the Dirac delta function of x in 3D for $x \in \mathbb{R}^3$ is defined by:

$$\delta(x) = \begin{cases} 0, & \text{for } x \neq 0 \\ \infty, & \text{for } x = 0 \end{cases}, \quad \int_{\Omega} \delta(x) dx = \begin{cases} 1, & \text{for } x \in \Omega \\ \infty, & \text{for } x \notin \Omega \end{cases}$$

3.4 Greens identities

Theorem 3.1 (Greens first identity, [50]) . Let $\Omega \subset \mathbb{R}^3$ be a domain bounded by the closed piecewise smooth boundary $\partial\Omega$ and let n denote the unit normal vector to the boundary $\partial\Omega$ directed into the exterior of $\partial\Omega$. Let $u, v \in C^2(\Omega)$, then

$$\int_{\Omega} (u\Delta v + \nabla u \cdot \nabla v) d\Omega = \int_{\partial\Omega} u \frac{\partial v}{\partial n} ds \quad (3.3)$$

Proof 3.1 By applying Gauss divergence theorem,

$$\int_{\Omega} \text{div} \vec{F} dV = \int_{\partial\Omega} \vec{F} \cdot \hat{n} dS \quad (3.4)$$

to the vector function (vector field) $F = (F_1, F_2) \in C^1(\Omega)$ (with the components) F_1, F_2 being once continuously differentiable in the closed domain Ω defined by

$$\vec{F} = u\nabla v = \left[u \frac{\partial v}{\partial x}, u \frac{\partial v}{\partial y} \right]$$

the components are, $\vec{F}_1 = u \frac{\partial v}{\partial x}$ and $\vec{F}_2 = u \frac{\partial v}{\partial y}$, we have

$$\begin{aligned} \operatorname{div} \vec{F} &= \operatorname{div}(u\nabla v) = \frac{\partial}{\partial x} \left(u \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(u \frac{\partial v}{\partial y} \right) \\ &= \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} + u \frac{\partial^2 v}{\partial x^2} + \frac{\partial u}{\partial y} \frac{\partial v}{\partial y} + u \frac{\partial^2 v}{\partial y^2} \\ &= \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial v}{\partial y} + u \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) = \nabla u \cdot \nabla v + u \nabla^2 v. \end{aligned}$$

Then taking the integral over Ω , we obtain,

$$\int_{\Omega} \operatorname{div} \vec{F} d\Omega = \int_{\Omega} (\nabla u \cdot \nabla v + u \nabla^2 v) d\Omega \quad (3.5)$$

On the other hand, according to the definition of the normal derivative

$$\vec{F} \cdot \hat{n} = (u\nabla v) \cdot \hat{n} = u(\nabla v \cdot \hat{n}) = u \frac{\partial v}{\partial n} \quad (3.6)$$

and from equation (3.6) and using equation (3.4) we have

$$\int_S \vec{F} \cdot \hat{n} dS = \int_S u \frac{\partial v}{\partial n} dS$$

Therefore,

$$\int_S u \frac{\partial v}{\partial n} ds = \int_{\Omega} (\nabla u \cdot \nabla v + u \Delta v) d\Omega$$

Theorem 3.2 (Greens second identity, [50]) For $u, v \in C^2(\Omega) \cap C^1(\bar{\Omega})$, the Greens second identity is given by,

$$\int_{\Omega} (u \Delta v - v \Delta u) d\Omega = \int_{\partial\Omega} \left(u \frac{\partial v}{\partial n} - v \frac{\partial u}{\partial n} \right) ds \quad (3.7)$$

Proof 3.2 By interchanging the role of u and v in the Greens first identity, (3.3), and subtracting the result, we get the result. The process by which (3.7) was derived from (3.3) is an example of symmetrization . This is Greens second identity and is a basic tool in the study of Δ .

3.5 BIE method for poisson equation with Dirichlet boundary condition

$$\begin{aligned} \Delta u &= f & \text{in } \Omega \\ u &= \bar{u} & \text{on } \partial\Omega \end{aligned} \quad (3.8)$$

This is the governing equation of potential theory, which for $f = 0$ is known as the Laplace equation, whereas for $f \neq 0$ is known as the Poisson equation. Its solution $u = u(p)$ represents the potential produced at a point Q in the domain Ω due to a source $f(p)$ distributed over Ω (see, figure:3.1). The potential equation (3.8) describes the response of many physical systems. It appears in steady state flow problems, such as fluid flow, thermal flow, electricity flow, as well as in torsion of prismatic bars, bending of membranes, etc. Its solution is sought in a closed plane domain Ω having a boundary $\partial\Omega$ on which either the function u or its derivative $\frac{\partial u}{\partial n}$ in the direction normal to $\partial\Omega$ is prescribed. That is, the solution must satisfy the boundary conditions of the problem on the boundary $\partial\Omega$.

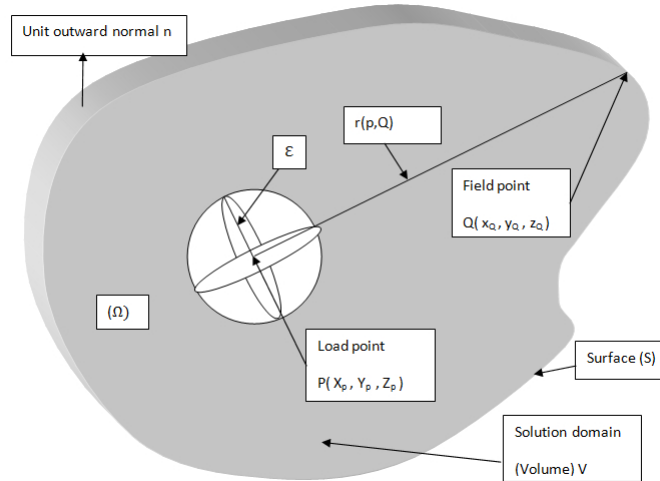


Figure 3.1: A three dimensional physical domain

Consider an arbitrary domain Ω where the solution is sought. In this solution domain, assume that there is an interior point p (usually called the 'load' point) of coordinates X_p, Y_p and Z_p and consider any point on the boundary Q (usually called the 'field' point) with coordinates x_Q, y_Q and z_Q . The use of capital letter for the coordinates indicates a fixed point, where as the lower case letters for the coordinates indicates a variable point (see Figure 3.1). The three dimensional fundamental solution of poisson equation based on a concentrated potential or source at point p can be easily varified as follows:

3.5.1 Fundamental solution

Let us consider a point source placed at point p . Its density at Q may be expressed mathematically by the delta function as[50]

$$f(Q) = \delta(Q - p)$$

and the potential $\lambda = \lambda(p, Q)$ produced at point Q satisfies the equation

$$\nabla^2 \lambda = \delta(Q - p). \quad (3.9)$$

Where the Dirac delta function denotes a unit source concentrated at the point p . No function has this property in fact it is a distribution rather than a function, but it can be thought of as a limit of function whose integrals over space are unity, and whose support (the region where the function is non-zero) shrinks to a point. It is common to take a different sign convention for this equation than one typically does when defining Fundamental solutions. This choice of sign is often convenient to work with because ∇^2 is a positive operator. The definition of the fundamental solution thus implies that, if the Laplacian of λ is integrated over any volume that incloses the source point, then

$$\iiint_V \nabla \cdot \nabla \lambda dV = 1.$$

The Laplace equation is unchanged under a rotation of coordinates, and hence we can expect that a fundamental solution may be obtained among solution that only depend up on the distance r from the source point. If we choose the volume to be a ball of radius r around the source point, then Gauss' divergence theorem implies that

$$\begin{aligned} 1 &= \iiint_V \nabla \cdot \nabla \lambda dV = \iint_S \frac{d\lambda}{dr} dS \\ &= 4\pi r^2 \frac{d\lambda}{dr} \end{aligned}$$

It follows that

$$\frac{d\lambda}{dr} = \frac{1}{4\pi r^2}$$

On a sphere of radius r that is centered on the source point, and hence

$$\lambda(p, Q) = \frac{1}{4\pi} \left[\frac{1}{r(p, Q)} \right] \quad (3.10)$$

Equation (3.10) is the Fundamental solution of poisson equation (3.9). Where $r(p, Q)$ is the distance between p and Q , given by

$$r(p, Q) = \sqrt{(X_p - x_Q)^2 + (Y_p - y_Q)^2 + (Z_p - z_Q)^2} \quad (3.11)$$

and the constant $\left(\frac{1}{4\pi}\right)$ is associated with the strength of the potential at the point p but can be considered arbitrary for the present purposes.

The solution of Eq.(3.8) can be obtained as a sum of two solutions

$$u = u_o + u_1 \quad (3.12)$$

where u_o is the solution of the homogeneous equation(3.8) and u_1 is a particular solution of the nonhomogeneous equation(3.8).

- (i) **Particular solution** (u_1) The particular solution of the non-homogeneous equation is any function u_1 that satisfies only the governing equation,

$$\nabla^2 u_1 = f, \quad (3.13)$$

independently of boundary condition. We will show next that

$$\begin{aligned} \nabla^2 u_1(p) &= f(p) \\ &= \int_{\Omega} \delta(Q-p) f(Q) d\Omega_Q \\ &= \int_{\Omega} \nabla^2 \lambda(Q,p) f(Q) d\Omega_Q \\ &= \nabla^2 \left[\int_{\Omega} \lambda(Q,p) f(Q) d\Omega_Q \right] \\ \nabla^2 \left[u_1(p) - \int_{\Omega} \lambda(Q,p) f(Q) d\Omega_Q \right] &= 0 \\ \Rightarrow u_1(p) &= \int_{\Omega} \lambda(Q,p) f(Q) d\Omega_Q \\ \Rightarrow u_1 &= \int_{\Omega} \lambda f d\Omega. \end{aligned}$$

Let us transform the domain integrals to boundary integrals

In this case f is an arbitrary source defined in Ω . We first establish an other function F which satisfies the following equation.

$$\nabla^2 F = f \quad (3.14)$$

The function F is determined as a particular solution of Eq.(3.14). The Green's identity is then applied for the function λ and F in the domain Ω .

$$\begin{aligned}
\int_{\Omega} (\lambda \nabla^2 F - F \nabla^2 \lambda) d\Omega &= \int_S \left(\lambda \frac{\partial F}{\partial n} - F \frac{\partial \lambda}{\partial n} \right) dS \\
\int_{\Omega} \lambda f d\Omega &= \int_{\Omega} F \nabla^2 \lambda d\Omega + \int_S \left(\lambda \frac{\partial F}{\partial n} - F \frac{\partial \lambda}{\partial n} \right) dS \\
&= \int_{\Omega} F \delta(Q - p) d\Omega_Q + \int_S \left(\lambda \frac{\partial F}{\partial n} - F \frac{\partial \lambda}{\partial n} \right) dS \\
u_1 &= \int_{\Omega} \lambda f d\Omega = F + \int_S \left(\lambda \frac{\partial F}{\partial n} - F \frac{\partial \lambda}{\partial n} \right) dS \\
u_1(p) &= F(p) + \int_S \left(\lambda(p, Q) \frac{\partial F(Q)}{\partial n} - F(Q) \frac{\partial \lambda(p, Q)}{\partial n} \right) dS. \quad (3.15)
\end{aligned}$$

To make this equation a truly 'boundary only' equation, we move the interior load point p to the boundary (refer to it as P) which results in the following equation:

$$u_1(P) = C(P)F(p) + \int_S \left(\lambda \frac{\partial F(Q)}{\partial n} - F(Q) \frac{\partial \lambda(Q)}{\partial n} \right) dS$$

Where $C(P)$ is a coefficient which depends on the position of point P and is defined as([50]):

$$C(P) = \begin{cases} 1 & \text{for } P \text{ inside } \Omega \\ \frac{1}{2} & \text{for } P \equiv p \text{ on the boundary } \partial\Omega \\ 0 & \text{for } P \text{ outside } \Omega \end{cases}$$

We take $C(P) = \frac{1}{2}$ because since we have considered smooth piecewise boundary.

ii Homogeneous solution u_o

$$\nabla^2 u_o = 0 \quad \text{in } \Omega \quad (3.16)$$

With the boundary condition

$$u_o = \bar{u} - u_1 \quad \text{on } \partial\Omega.$$

We assume the existence of two continuous mathematical function u_o and λ , that have continuous first and second derivative. u_o is function at any point, while λ is the three dimensional fundamental solution of Laplace's equation(3.10). Applying Green's theorem to these two function results in the following transformation from a volume integral dV to a surface integral dS :

$$\int_V (u_o \nabla^2 \lambda - \lambda \nabla^2 u_o) dV = \int_S \left(u_o \frac{\partial \lambda}{\partial n} - \lambda \frac{\partial u_o}{\partial n} \right) dS \quad (3.17)$$

where n is the unit outward normal. u_o satisfies $\nabla^2 u_o = 0$ every where in the solution domain. The fundamental solution λ , however, satisfies $\nabla^2 \lambda = 0$ everywhere except at the point p

where it is singular. To deal with this problem, we can surround the point p by a very small sphere of radius ε and surface S_ε , and examine the solution in the limit as $\varepsilon \rightarrow 0$. By excluding this small sphere, the new volume $(V - V_\varepsilon)$ and the new surface is $(S + S_\varepsilon)$, and Eq.(3.17) becomes

$$\int_{V-V_\varepsilon} (u_o \nabla^2 \lambda - \lambda \nabla^2 u_o) dV = \int_{S+S_\varepsilon} \left(u_o \frac{\partial \lambda}{\partial n} - \lambda \frac{\partial u_o}{\partial n} \right) dS \quad (3.18)$$

With the volume $(V - V_\varepsilon)$, $\nabla^2 u_o = 0 = \nabla^2 \lambda$ everywhere, which makes the left-hand side equal to zero, and the surface integral $(S + S_\varepsilon)$ can now be split into two surface integrals resulting in the following equation:

$$0 = \int_S \left(u_o \frac{\partial \lambda}{\partial n} - \lambda \frac{\partial u_o}{\partial n} \right) dS + \int_{S_\varepsilon} \left(u_o \frac{\partial \lambda}{\partial n} - \lambda \frac{\partial u_o}{\partial n} \right) dS \quad (3.19)$$

Referring the sphere centred at p , the second integral in Eq.(3.19) can be written as follows:

$$\int_0^\pi \left(u_o \frac{\partial \lambda}{\partial n} - \lambda \frac{\partial u_o}{\partial n} \right) 2\pi \varepsilon^2 \sin \alpha d\alpha \quad (3.20)$$

where α is the angle measured anticlockwise from the x -axis at point p . Substituting for λ Eq.(3.10) and using $\frac{\partial}{\partial n} = -\frac{\partial}{\partial r}$ on the surface S_ε , the integral of Eq.(3.20) becomes

$$\begin{aligned} & \int_0^\pi \left[u_o(p) \frac{\partial}{\partial n} \left(\frac{1}{4\pi r} \right) - \left(\frac{1}{4\pi r} \right) \frac{\partial u_o}{\partial n} \right] 2\pi \varepsilon^2 \sin \alpha d\alpha \\ &= \int_0^\pi \left[u_o(p) \left(\frac{1}{4\pi \varepsilon^2} \right) - \left(\frac{1}{4\pi \varepsilon} \right) \frac{\partial u_o}{\partial n} \right] 2\pi \varepsilon^2 \sin \alpha d\alpha \end{aligned} \quad (3.21)$$

Taking each term in the limit as $\varepsilon \rightarrow 0$ result in the following:

$$\frac{1}{2} u_o(p) \int_0^\pi \sin \alpha d\alpha = \frac{1}{2} u_o(p) [-\cos \alpha]_0^\pi d\alpha = u_o(p) \quad (3.22)$$

Substituting this result in Eq.(3.19) and rearranging the terms results in the following boundary integral equation(BIE):

$$u_o(p) = - \int_S \left(u_o(Q) \frac{\partial \lambda}{\partial n} - \lambda \frac{\partial u_o(Q)}{\partial n} \right) dS \quad (3.23)$$

To make this equation a truly 'boundary only' equation, we move the interior load point p to the boundary (refer to it as P) which results in the following equation:

$$C(P) u_o(P) = - \int_S \left(u_o(Q) \frac{\partial \lambda}{\partial n} - \lambda \frac{\partial u_o(Q)}{\partial n} \right) dS$$

Where $C(P)$ is a coefficient which depends on the position of point P and is defined as([50]):

$$C(P) = \begin{cases} 1 & \text{for } P \text{ inside } \Omega \\ \frac{1}{2} & \text{for } P \equiv p \text{ on the boundary } \partial\Omega \\ 0 & \text{for } P \text{ outside } \Omega. \end{cases}$$

We take $C(P) = \frac{1}{2}$ because since we have considered smooth picewice boundary. Now adding Eq.(3.15) and Eq.(3.23) We get the general solution for u (3.12)as follows:-

$$u(P) = \frac{1}{2}F(P) + \int_S \left(\lambda \frac{\partial F(Q)}{\partial n} - F(Q) \frac{\partial \lambda}{\partial n} \right) dS - 2 \int_S \left(u_o(Q) \frac{\partial \lambda}{\partial n} - \lambda \frac{\partial u_o(Q)}{\partial n} \right) dS. \quad (3.24)$$

Chapter 4

Analysis of Heat flow in Resistive Switching Devices

4.1 Problem Formulation

We consider a three-layered device of lateral dimensions l_x and l_y , where it is illustrated schematically in the Figure 4.1. Let the metal electrodes have thicknesses of t_1 and t_3 and the insulator has thickness h .

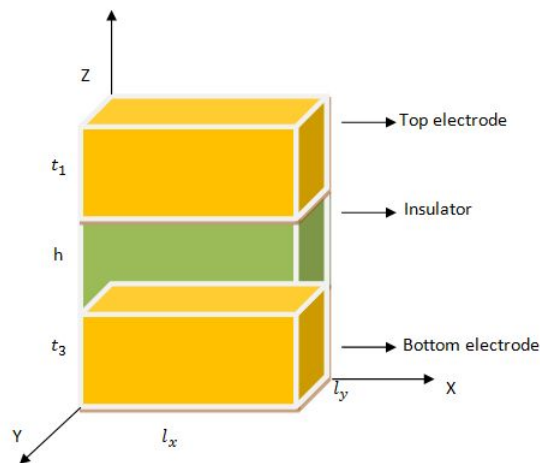


Figure 4.1: The Composite device in space

Geometrically the region of interest can be described by a domain $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3$, where

$$\begin{aligned}\Omega_1 &= \{(x, y, z) : 0 < x < l_x, 0 < y < l_y, t_3 + h < z < t_3 + h + t_1\} \\ \Omega_2 &= \{(x, y, z) : 0 < x < l_x, 0 < y < l_y, t_3 < z \leq t_3 + h\} \\ \Omega_3 &= \{(x, y, z) : 0 < x < l_x, 0 < y < l_y, 0 < z \leq t_3\}\end{aligned}$$

Let $T_i(x, y, z)$, $i = 1, 2, 3$ be the temperature profile in the two electrodes and in the insulator with k_i , $i = 1, 2, 3$ are corresponding thermal conductivity. In each layer the heat equation is given by

$$\nabla \cdot (k_i \nabla T_i) = -S_i(x, y, z). \quad (4.1)$$

where $S_i(x, y, z)$, $i = 1, 2, 3$ arbitrary source of power-density profile in the electrodes and insulator. We assume that there is no heat source in the two electrodes, i.e., $S_1 = S_3 = 0$. We analyze and describe the heat profile in the device with Dirichlet boundary conditions. We impose zero-temperature boundary condition $T(x, y, z) = 0$ at the outer edges of each layer, i.e., at $x = 0$ and $l_x = 0$ and l_y .

4.2 Formulation of Boundary Integral Equation for the Resistive Switching Devices

In this section, using the integral representation formula, we formulate the integral expression of the heat profile for each layers separately.

The Top electrode

The First layer or the top electrode occupies the region in $\mathbb{R}^3$ given by

$\Omega_1 = \{(x, y, z) : 0 < x < l_x, 0 < y < l_y, t_3 + h < z < t_3 + h + t_1\}$ (see, Fig 4.2)

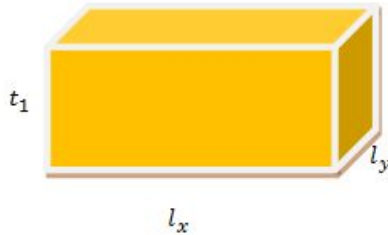


Figure 4.2: Top electrode

The temperature $T_1(x, y, z)$ satisfies the heat equation

$$\Delta T_1 = 0 \quad \text{in } \Omega_1. \quad (4.2)$$

For $p_1 \in \Omega_1$, applying the second Green's identity (3.23), we get the boundary integral equation,

$$T_1(p_1) + \int_{\partial\Omega_1} \frac{\partial\lambda(p_1, Q)}{\partial n} T_1(Q) dS(Q) = \int_{\partial\Omega_1} \lambda(p_1, Q) \frac{\partial T_1(Q)}{\partial n} dS(Q). \quad (4.3)$$

If we move the interior load point $p_1 \in \partial\Omega_1$ to the boundary pint $P_1 \in \partial\Omega_1$,

$$\frac{1}{2} T_1(P_1) + \int_{\partial\Omega_1} \frac{\partial\lambda(P_1, Q)}{\partial n} T_1(Q) ds(Q) = \int_{\partial\Omega_1} \lambda(P_1, Q) \frac{\partial T_1(Q)}{\partial n} ds(Q). \quad (4.4)$$

The Insulator

The region $\mathbb{R}^3$ occupied by the insulator, shown in the Figure (4.3), is given by,

$$\Omega_2 = \{(x, y, z) : 0 < x < l_x, 0 < y < l_y, t_3 < z < t_3 + h\}$$

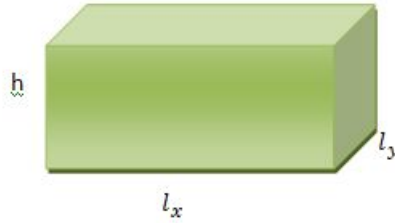


Figure 4.3: Insulator

The temperature $T_2(x, y, z)$ satisfies the heat equation

$$\Delta T_2 = -\frac{1}{k_2} S_2(x, y, z) \quad \text{in } \Omega_2. \quad (4.5)$$

The application of the representation formula (3.15) yields the integral equation for $p_2 \in \Omega_2$,

$$T_2(p_2) + \int_{\partial\Omega_2} \frac{\partial\lambda(p_2, Q)}{\partial n} T_2(Q) dS(Q) = \int_{\partial\Omega_2} \lambda(p_2, Q) \frac{\partial T_2(Q)}{\partial n} dS(Q) + \frac{1}{k_2} \int_{\Omega} S_2(p_2, Q) \lambda(p_2, Q) d\Omega. \quad (4.6)$$

If we move the interior load point $p_2 \in \partial\Omega_2$ to the boundary pint $P_2 \in \partial\Omega_2$,

$$\frac{1}{2} T_2(P_2) + \int_{\partial\Omega_2} \frac{\partial\lambda(P_2, Q)}{\partial n} T_2(Q) dS(Q) = \int_{\partial\Omega_2} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} dS(Q) + \frac{1}{k_2} \int_{\Omega} S_2(P_2, Q) \lambda(P_2, Q) d\Omega. \quad (4.7)$$

Bottom electrode

Similarly, the bottom electrode occupies the region $\mathbb{R}^3$ given by (see, Fig: 4.4)

$$\Omega_3 = \{(x, y, z) : 0 < x < l_x, 0 < y < l_y, 0 < z < t_3\}$$

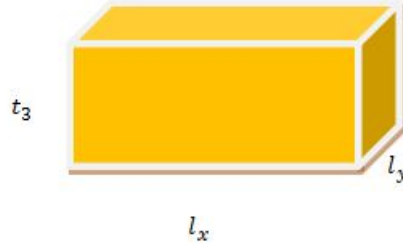


Figure 4.4: Botom electrod

The temperature $T_3(x, y, z)$ satisfies the heat equation

$$\Delta T_3 = 0 \quad \text{in } \Omega_3. \quad (4.8)$$

For $p_3 \in \Omega_3$, applying the second Green's identity (3.23), we get the boundary integral equation,

$$T_3(p_3) + \int_{\partial\Omega_3} \frac{\partial\lambda(p_3, Q)}{\partial n} T_3(Q) dS(Q) = \int_{\partial\Omega_3} \lambda(p_3, Q) \frac{\partial T_3(Q)}{\partial n} dS(Q). \quad (4.9)$$

If we move the interior load point $p_3 \in \partial\Omega_3$ to the boundary pint $P_3 \in \partial\Omega_3$,

$$\frac{1}{2} T_3(P_3) + \int_{\partial\Omega_3} \frac{\partial\lambda(P_3, Q)}{\partial n} T_3(Q) dS(Q) = \int_{\partial\Omega_3} \lambda(P_3, Q) \frac{\partial T_3(Q)}{\partial n} dS(Q). \quad (4.10)$$

Let Γ_1 be the common boundary between the top electrode and the insulator while Γ_2 be the common boundary between the bottom electrode and the insulator. Now imposing the Dirichlet boundary conditions, from the boundary integral equation (4.4), we have

$$\frac{1}{2} T_1(P_1)|_{\Gamma_1} + \int_{\Gamma_1} \frac{\partial\lambda(P_1, Q)}{\partial n} T_1(Q) ds(Q) = \int_{\partial\Omega_1} \lambda(P_1, Q) \frac{\partial T_1(Q)}{\partial n} ds(Q), \quad (4.11)$$

$$\frac{1}{2} T_1(P_1)|_{\Gamma_1} + \int_{\Gamma_1} \frac{\partial\lambda(P_1, Q)}{\partial n} T_1(Q) ds(Q) = \int_{\Gamma_1 \cup (\partial\Omega_1 \setminus \Gamma_1)} \lambda(P_1, Q) \frac{\partial T_1(Q)}{\partial n} ds(Q),$$

$$\frac{1}{2} T_1(P_1)|_{\Gamma_1} + \int_{\Gamma_1} \frac{\partial\lambda(P_1, Q)}{\partial n} T_1(Q) ds(Q) = \int_{\Gamma_1} \lambda(P_1, Q) \frac{\partial T_1(Q)}{\partial n} ds(Q) + \int_{\partial\Omega_1 \setminus \Gamma_1} \lambda(P_1, Q) \frac{\partial T_1(Q)}{\partial n} ds(Q). \quad (4.12)$$

From the boundary integral equation (4.7), we have

$$\frac{1}{2}T_2(P_2)|_{\Gamma_1 \cup \Gamma_2} + \int_{\Gamma_1 \cup \Gamma_2} \frac{\partial \lambda(P_2, Q)}{\partial n} T_2(Q) ds(Q) = \int_{\partial \Omega_2} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} ds(Q) + \frac{1}{k_2} \int_{\Omega} S_2(P_2, Q) \lambda(P_2, Q) d\Omega, \quad (4.13)$$

$$\begin{aligned} \frac{1}{2}T_2(P_2)|_{\Gamma_1 \cup \Gamma_2} + \int_{\Gamma_1 \cup \Gamma_2} \frac{\partial \lambda(P_2, Q)}{\partial n} T_2(Q) ds(Q) \\ = \int_{(\Gamma_1 \cup \Gamma_2) \cup (\partial \Omega_2 \setminus (\Gamma_1 \cup \Gamma_2))} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} ds(Q) + \frac{1}{k_2} \int_{\Omega} S_2(P_2, Q) \lambda(P_2, Q) d\Omega, \end{aligned}$$

$$\begin{aligned} \frac{1}{2}T_2(P_2)|_{\Gamma_1 \cup \Gamma_2} + \int_{\Gamma_1} \frac{\partial \lambda(P_2, Q)}{\partial n} T_2(Q) ds(Q) + \int_{\Gamma_2} \frac{\partial \lambda(P_2, Q)}{\partial n} T_2(Q) ds(Q) = \int_{(\Gamma_1 \cup \Gamma_2)} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} ds(Q) \\ + \int_{(\partial \Omega_2 \setminus (\Gamma_1 \cup \Gamma_2))} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} ds(Q) + \frac{1}{k_2} \int_{\Omega} S_2(P_2, Q) \lambda(P_2, Q) d\Omega, \end{aligned}$$

$$\begin{aligned} \frac{1}{2}T_2(P_2)|_{\Gamma_1 \cup \Gamma_2} + \int_{\Gamma_1} \frac{\partial \lambda(P_2, Q)}{\partial n} T_2(Q) ds(Q) + \int_{\Gamma_2} \frac{\partial \lambda(P_2, Q)}{\partial n} T_2(Q) ds(Q) = \int_{\Gamma_1} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} ds(Q) \\ + \int_{\Gamma_2} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} ds(Q) + \int_{(\partial \Omega_2 \setminus (\Gamma_1 \cup \Gamma_2))} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} ds(Q) + \frac{1}{k_2} \int_{\Omega} S_2(P_2, Q) \lambda(P_2, Q) d\Omega. \end{aligned} \quad (4.14)$$

And from the boundary integral equation (4.10), we have

$$\frac{1}{2}T_3(P_3)|_{\Gamma_2} + \int_{\Gamma_2} \frac{\partial \lambda(P_3, Q)}{\partial n} T_3(Q) ds(Q) = \int_{\partial \Omega_3} \lambda(P_3, Q) \frac{\partial T_3(Q)}{\partial n} ds(Q), \quad (4.15)$$

$$\frac{1}{2}T_3(P_3)|_{\Gamma_2} + \int_{\Gamma_2} \frac{\partial \lambda(P_3, Q)}{\partial n} T_3(Q) ds(Q) = \int_{\Gamma_2 \cup (\partial \Omega_3 \setminus \Gamma_2)} \lambda(P_3, Q) \frac{\partial T_3(Q)}{\partial n} ds(Q),$$

$$\frac{1}{2}T_3(P_3)|_{\Gamma_2} + \int_{\Gamma_2} \frac{\partial \lambda(P_3, Q)}{\partial n} T_3(Q) ds(Q) = \int_{\Gamma_2} \lambda(P_3, Q) \frac{\partial T_3(Q)}{\partial n} ds(Q) + \int_{(\partial \Omega_3 \setminus \Gamma_2)} \lambda(P_3, Q) \frac{\partial T_3(Q)}{\partial n} ds(Q), \quad (4.16)$$

Let

$$\begin{aligned} \varphi_1 &= T_1|_{\Gamma_1} = T_2|_{\Gamma_1}, \\ \varphi_2 &= T_2|_{\Gamma_2} = T_3|_{\Gamma_2} \quad \text{and} \\ \psi_1 &= \frac{\partial T_1}{\partial n}|_{\Gamma_1} = \frac{\partial T_2}{\partial n}|_{\Gamma_1}, \\ \psi_2 &= \frac{\partial T_2}{\partial n}|_{\Gamma_2} = \frac{\partial T_3}{\partial n}|_{\Gamma_2}. \end{aligned}$$

From the boundary integral equation (4.12), we have

$$\frac{1}{2}\phi_1 + \int_{\Gamma_1} \frac{\partial \lambda(P_1, Q)}{\partial n} \phi_1 ds(Q) = \int_{\Gamma_1} \lambda(P_1, Q) \psi_1 ds(Q) + \int_{\partial\Omega_1 \setminus \Gamma_1} \lambda(P_1, Q) \frac{\partial T_1(Q)}{\partial n} ds(Q). \quad (4.17)$$

From the boundary integral equation (4.16), we have

$$\frac{1}{2}\phi_2 + \int_{\Gamma_2} \frac{\partial \lambda(P_1, Q)}{\partial n} \phi_2 ds(Q) = \int_{\Gamma_2} \lambda(P_1, Q) \psi_2 ds(Q) + \int_{\partial\Omega_3 \setminus \Gamma_2} \lambda(P_1, Q) \frac{\partial T_1(Q)}{\partial n} ds(Q). \quad (4.18)$$

And from the boundary integral equation (4.14), we have

$$\begin{aligned} \frac{1}{2}\phi_1 + \frac{1}{2}\phi_2 + \int_{\Gamma_1} \frac{\partial \lambda(P_2, Q)}{\partial n} \phi_1 ds(Q) + \int_{\Gamma_2} \frac{\partial \lambda(P_2, Q)}{\partial n} \phi_2 ds(Q) &= \int_{\Gamma_1} \lambda(P_2, Q) \psi_1 ds(Q) \\ &+ \int_{\Gamma_2} \lambda(P_2, Q) \psi_2 ds(Q) + \int_{(\partial\Omega_2 \setminus (\Gamma_1 \cup \Gamma_2))} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} ds(Q) + \frac{1}{k_2} \int_{\Omega} S_2(P_2, Q) \lambda(P_2, Q) d\Omega. \end{aligned} \quad (4.19)$$

By substituting equation 4.17 and 4.18 in equation 4.19 and simplifying we get

$$\begin{aligned} \frac{1}{k_2} \int_{\Omega} S_2(P_2, Q) \lambda(P_2, Q) d\Omega &= \int_{\partial\Omega_1 \setminus \Gamma_1} \lambda(P_1, Q) \frac{\partial T_1(Q)}{\partial n} ds(Q) + \int_{\partial\Omega_3 \setminus \Gamma_2} \lambda(P_1, Q) \frac{\partial T_1(Q)}{\partial n} ds(Q) \\ &- \int_{(\partial\Omega_2 \setminus (\Gamma_1 \cup \Gamma_2))} \lambda(P_2, Q) \frac{\partial T_2(Q)}{\partial n} ds(Q). \end{aligned} \quad (4.20)$$

Chapter 5

Conclusion

We have formulated the boundary integral equation for each layer(the temperature profile in a metal-insulator-metal structure with multiple cuboidal heat sources within the insulator). And we have analyzed the Boundary Integral Equation(BIE) methods for the poisson equation with Dirichlet Boundary Conditions in three dimensions where the boundary is smooth. We presented a formulation of solving the BIEs reformulated from the poisson boundary value problems. A boundary value problem for Partial Differential Equation with a constant coefficient can be reduced to a BIE by using the fundamental solution and Greens representation formula, we have reduced the boundary value problem into Boundary Integral Equations. Boundary integral equation Method is developed for the problem of heat conduction in a geometry composed of an insulator between two metallic electrodes, with multiple cuboidal heat sources within the insulator.

We hope that this thesis will inspire more work in the future in this area.

References

- [1] T.W. Hickmott, J.(1962) .Applied Physics.
- [2] Weinberg and S. (2015). “The Discovery of Subatomic Particles” Revised Edition. Cambridge University Press.
- [3] Perry, R. H. Green, D. W.(1997), “Perry’s Chemical Engineers’ Handbook”, 7th ed.
- [4] Aliabadi. M.H.(2002). The Boundary Element Method, Applications in Solids and Structures. Wiley, Chichester, Vol. 2
- [5] Kleinman. R.E. and Roach. G.F.(1974) , Boundary integral equations for the three-dimensional Helmholtz equation, SIAM, Review, Vol. 16, 217-219.
- [6] Schenck, H. A. (1968), Improved integral formulation for acoustics radiation problems, J. Acoust. Soc. Am., 44, 41-58.
- [7] William J. Parnell (2013), Greens functions, integral equations and applications,
- [8] D. B. Strukov and R. S. Williams,(2009). “Exponential ionic drift: Fast switching and low volatility of thin film memristors,”Appl. Phys. A, vol. 94, no. 3, pp. 515-519,
- [9] S. Larentis, F. Nardi, and S. Balatti,(2012) “Resis- tive switching by voltage-driven ion migration in bipolar RRAM Part II: Modeling,” IEEE Trans. Electron Devices, vol. 59, no. 9, pp. 2468-2475, Sep.
- [10] U. Russo, D. Ielmini, and C. Cagli,(2007) “Conductive-filament switching analysis and self-accelerated thermal dissolution model for reset in NiO- based RRAM,” in Proc. Int. Electron Devices Meeting, pp. 775-778.
- [11] J. L. Borghetti, D. M. Strukov, and M. D. Pickett,(2009) “Electrical transport and thermometry of electroformed titanium dioxide memristive switches,” J. Appl. Phys., vol. 106, no. 12.
- [12] S. H. Chang, S. C. Chae, and S. B. Lee,(2008) “Effects of heat dissipation on unipolar resistance switching in Pt/NiO/Pt capacitors,” Appl. Phys. Lett., vol. 92, no. 18.
- [13] A. Shkabko, M. H. Aguirre, and I. Marozau,(2009) “Measurements of current voltage induced heating in the memristor during electroformation and resistance switching,” Appl. Phys. Lett., vol. 95, no. 15.

- [14] J. P. Strachan, D. B. Strukov, and J. Borghetti, (2011)“The switching location of a bipolar memristor: Chemical, thermal and structural mapping,” *Nanotechnology*, vol. 22, no. 25.
- [15] N. A. Tulina and V. V. Sirotkin (2004)“Electron instability in dopedmanganites based heterojunctions,” *Phys. C, Supercond.*, vol. 400, nos. 3-4, pp. 105-110.
- [16] C. L. Tan, R. T. Fenner (1979) “Stress intensity factors for semi-elliptical surface cracks in pressurised cylinders using the boundary integral equation method”.
- [17] L.S. Xanthis, M.J.M. Bernal, C. Atkinson (1981) “The treatment of singularities in the calculation of stress intensity factors using the boundary integral equation method”.
- [18] G.Bezine (1981) used a boundary integral equation method for plate flexure with conditions inside the domain.
- [19] Katsikadelis, J. T., Armenakas, A. E.(1984) “Analysis of Clamped Plates on Elastic Foundation by the Boundary Integral Equation Method” .
- [20] AbdulMihsein, M.J., Bakr, A.A., Fenner, R.T.(1985) “Stress analysis of pressure vessels and piping using the boundary integral equation method”.
- [21] F. J. Rizzo,D. J. Shippy and M. Rezayat (1985) “A boundary integral equation method for radiation and scattering of elastic waves in three dimensions”.
- [22] M. Kitahara (1985) “Boundary Integral Equation Methods in Eigenvalue Problems of Elastodynamics and Thin Plates”.
- [23] David L. Clements, M. Haselgrove (1985) “The boundary integral equation method for the solution of problems involving elastic slabs”.
- [24] LEE, K H, FENNER, R T (1986)“A quadratic formulation for two-dimensional elastoplastic analysis using the boundary integral equation method”.
- [25] G. Karami, R. T. Fenner (1986)“Analysis of mixed mode fracture and crack closure using the boundary integral equation method”.
- [26] Ishibashi, K., Sawado, E.(1990) “Three-dimensional analysis of electromagnetic fields in rectangular waveguides by the boundary integral equation method”.
- [27] ERMAN, Z, FENNER, R T (1996) “Three-dimensional design optimization using the boundary integral equation method”.
- [28] K. TAI, R. T. FENNER (1996) “Optimum shape design and positioning of features using the boundary integral equation method”.
- [29] M. J. BLUCK, S. P. WALKER (1996) “Analysis of three dimentional transient acoustic wave propagation using boundary integral equation method”.
- [30] David Natroshvili(1997) “Boundary Integral Equation Method in the Steady State Oscillation Problems for Anisotropic Bodies”.

- [31] LIU, ENRU, ZHANG, ZHONGJIE (2000) “numerical study of elastic wave scattering by cracks or inclusions using the boundary integral equation method”.
- [32] M.P. Savruk, S.V. Shkarayev (2001) “Stress singularities for three-dimensional corners using the boundary integral equation method”.
- [33] E. E. Theotokoglou (2003) “Boundary integral equation method to solve embedded planar crack problems under shear loading”.
- [34] S. Orlowska, A. Beroual, J. Fleszynski (2004) “A boundary integral equation method in the prediction of dielectric characteristics of humidified composite insulator glass epoxy core”.
- [35] C. Y. Dong, Kang Yong Lee (2005) “Numerical analysis of doubly periodic array of cracks/rigid-line inclusions in an infinite isotropic medium using the boundary integral equation method”.
- [36] J. T. Chen, C. S. Wu, K. H. Chen, Y. T. Lee (2006) “Degenerate scale for the analysis of circular thin plate using the boundary integral equation method and boundary element methods”.
- [37] A. K. Alexandrov, I. S. Yatchev (2007) “Permeance computation using the boundary integral equation method”.
- [38] David L. Clements and Oscar A. C. Jones (2009) “The boundary integral equation method for the solution of a class of problems in anisotropic elasticity”.
- [39] Iraj Mantegh, Michael R. M. Jenkin, Andrew A. Goldenberg (2010) “Path Planning for Autonomous Mobile Robots Using the Boundary Integral Equation Method”.
- [40] Menshykova, M. V., Menshykov, O. V., Guz, I. A., Wuensche, M., Zhang, Ch. (2016) “A boundary integral equation method in the frequency domain for cracks under transient loading”.
- [41] Talaat Osman and A.B. (2009) “Analytical solution for the 3D steady state conduction in a solid subjected to a moving rectangular heat source and surface cooling”.
- [42] Cheng Rong-Jun and Ge Hong-Xia (2010) “numerical solution of three-dimensional steady-state heat conduction problems”.
- [43] Tao Nie, Weiqiang Liu (2012) “Analytical Solutions of Three Dimensional Steady-State Heat Transfer in Rectangular Ribs”.
- [44] dott. Ing. Bulut Ilemisli (2015) “Analytical solutions of the steady or unsteady heat conduction equation in industrial devices: A comparison with FEM results”.
- [45] Cheng, A. H.D.; Cheng, D. T. (1992) “Heritage and early history of the boundary element method”.
- [46] W. A. Strauss. (1992) *Partial Differential Equations: An Introduction*. New York, NY, USA: John Wiley and Sons.

- [47] Nakle H.Asmar (2004) Partial Differential Equation with Fourier series and Boundery value problems Second edition.
- [48] PETER V.O'NEIL. (2012) Advanced Enginering Mathematics seventh edition.
- [49] Alberto Bressan.(2013) Lecture notes on functional analysis with applications to linear partial differential equations. American Mathematical Society.
- [50] John T.Katsikadelis.(2002) Boundery elements:Theory and Applications.
- [51] Wolfgang Hackbusch.(1995) Integral equation Theory and Numerical treatment. Birkhauser Verlag: Switzerland, 1st edition.