ELECTRIC FIELD MODELLING OF POLYMER NANOCOMPOSITES UNDER VARIOUS NANOPARTICLES DISTRIBUTIONS

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DEDICATION

Oh My Lord, increase me in knowledge

(Quran 20:114)

To my beloved family and friends

ACKNOWLEDGEMENT

In the name of Allah, The Most Gracious and The Most Merciful.

First and foremost, I am expressing my appreciation and praise to God the Almighty for His guidance and blessings throughout my entire study in University Technology of Malaysia.

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ABSTRACT

High voltage insulators play an important role in electrical power transmission systems. The insulators not only function as dielectric materials, but also need to meet other specifications, which includes mechanical, thermal and economic requirements. Most of the electrical insulators are made of glasses, porcelains and ceramics, but the insulators may fail to operate under large electrical fields due to electrical breakdown. Recently, nanocomposites have been developed as a novel insulation system that provide significantly improved electrical, thermal, mechanical and chemical properties. In terms of dielectric properties, the use of nanofillers leads to a high volume fraction of the interaction zones between the particles and polymer matrix called interphase. However, many studies of nanocomposites have assumed that nanofillers are homogeneously dispersed and their interphases are uniform in size. With the increasing availability and reducing cost of computers, numerical techniques in Finite Element Method Magnetics (FEMM) 4.2 software have become one of the popular tools for calculating electrical field distribution. To carry out a simulation study on the effect of nanoparticle interphase in polymer nanocomposites, the current work has considered an interphase model based on polymer and nanoparticle with fixed permittivity. To determine the effects of electric field distribution in relation to the non-homogeneous nanoparticle dispersion, changes in the models have been determined by varying nanoparticles size, the interphase thickness, the permittivity values within interphase and the position of nanoparticles.

ABSTRAK

Penebat voltan tinggi memainkan peranan yang penting dalam sistem penghantaran tenaga elektrik. Penebat bukan sahaja berfungsi sebagai material dielektrik namun perlu memenuhi spesifikasi lain dan ini termasuklah keperluan mekanikal, terma serta ekonomi. Kebanyakan penebat elektrik diperbuat daripada gelas, porselin dan seramik, tetapi penebat mungkin gagal berfungsi di bawah medan elektrik yang besar disebabkan kerosakan elektrik. Sejak kebelakangan ini, nanokomposit telah dibangunkan sebagai sistem penebat baru yang menyebabkan penambahbaikan yang signifikan dari segi elektrik, haba, mekanikal dan kimia. Dari segi sifat dielektrik, partikel nano menghasilkan zon interaksi antara partikel dan polimer yang dikenali sebagai ‘interphase’. Walau bagaimanapun, banyak kajian yang dijalankan mengenai nanokomposit mengandaikan bahawa partikel nano disebarkan secara homogen dan ‘interphase’ adalah bersaiz seragam. Dengan peningkatan ketersediaan dan pengurangan kos komputer, teknik berangka dalam perisian Finite Element Method Magnetics (FEMM) 4.2 telah menjadi salah satu perisian yang terkenal untuk mengira pengagihan medan elektrik. Untuk menjalankan kajian simulasi mengenai kesan ‘interphase’ partikel nano dalam polimer nanokomposit, model ‘interphase’ yang dipertimbangkan untuk simulasi ini adalah berdasarkan pada polimer dan partikel nano yang mempunyai nilai permitiviti yang malar. Untuk menentukan kesan pengagihan medan elektrik berhubung dengan pengagihan partikel nano yang tidak homogen, perubahan dalam model ditentukan oleh pelbagai saiz partikel nano, ketebalan dan nilai permittiviti dalam ‘interphase’ serta kedudukan partikel nano dalam polimer nanokomposit.

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LIST OF ABBREVATIONS

HVAC	-	High Voltage Alternating Current
HVDC	-	High Voltage Direct Current
FEMM 4.2	-	Finite Element Method Magnetics 4.2
CNT	-	Carbon nanotubes
DC	-	Direct Current
nn	-	Nearest neighbour
µm	-	micrometre
nm	-	nanometre
TiO_2	-	Titanium Dioxide
$CaCO_3$	-	Calcium Carbonate
Al_2O_3	-	Alumina
BT	-	Barium Titanate
SiO_2	-	Silica Dioxide
PE	-	Polyethylene
NP	-	Nanoparticle
IP	-	Interphase
vs	-	Versus

LIST OF SYMBOLS

wt%	-	Weight Percentage
ε_r	-	Permittivity value
kV	-	Kilo Volts
kV/mm	-	Kilo Volts per millimetre

CHAPTER 1

INTRODUCTION

1.1 Background of Project

Dielectric materials with high breakdown strength are beneficial for high voltage and large capacity as well as miniaturized power equipment and electronic devices. The interest in polymer nanocomposites at engineering level started when polyamide 6/clay nanocomposite was manufactured as engineering plastics on a commercial basis in 1990. This achievement initiated research and development efforts to investigate the possibility of combination of various polymers with various nano-inorganic fillers. While nanotechnology has been utilized in the semiconductor, biological and sensor arenas, utilization of the technology in insulation system has been slow to be developed. However, the year 1994 becomes a turning point in dielectrics and electrical insulation field, when John Lewis published a revolutionary theoretical paper, 'Nanometric Dielectrics' in the IEEE Transactions on Dielectrics and Electrical Insulation as future research area of dielectrics. The tendency toward nanodielectric research attracted worldwide interest after Nelson et al. highlighted new experimental work in 2002 with the emerging need of power engineers to design new electrical insulation systems that are capable of withstanding higher voltage levels, such as those for HV alternating current (HVAC) and HV direct current (HVDC) applications [1].

The incorporation of nanoparticles into polymer is an effective approach to improve its electrical breakdown performance. Recent studies showed that the use of nanofillers in polymeric insulating materials can lead to enhanced properties compared to microfilled and unfilled materials. The use of nanoscale filler in polymers can improve electrical breakdown strength and possesses a higher resistance to surface discharges and treeing, a reduction of accumulation of space charge, a higher resistance to electrical treeing, a higher resistance to water treeing, an improved thermal endurance and an improved thermal conductivity [1]. Besides, nanofillers provide advantages over microfillers because they provide resistance to degradation and improvement in thermo-mechanical properties without causing a reduction in dielectric strength [8].

Polymer nanocomposites can be distinguished from microcomposites in three major aspects. First, the difference in filler content. Conventional micro-sized filler composites usually consist of a large amount of more than 50wt% of fillers hence mixture of polymer with mineral filler resulting in a tremendous change of polymer properties. Meanwhile, nanocomposites contains much smaller amount of filler which is 10wt% or less so that some intrinsic polymeric properties remain almost unchanged even after becoming resulting material of the nanocomposites. Second, the size of the filler itself, where micro-sized fillers are used in micro composites and nanofiller sized fillers are used in nanocomposites. Third, nanocomposites have larger area surface compared to microcomposites. These differences are summarized in Table 1.1.

Table 1.1 Comparison between microcomposites and nanocomposites

Parameters	**Microcomposites**	**Nanocomposites**
Filler size (m)	10^{-6}	10^{-9}
Filler content (wt%)	> 50	< 10
Filler surface area	Small	Large

On the other hand, the enhancement properties due to the use of nanoparticle filler lead to a modification of macroscopic material properties which is attributed to the high volume fraction of the interaction zones between the particles and the polymer matrix called interphase. In addition, these interaction areas can have different structures and properties compared to the surrounding polymer and the filler particles.

Nevertheless, polymer nanocomposites will also suffer from breakdown failures, which is the similar mechanism that leads to failure in the pure polymers and microcomposites. With the aim to clearly understand the role of the interphase in nanocomposites, it is significant to study the effect of the interphase behavior on the electric field distribution in nanocomposites. Many models have been proposed to explain the interphase areas since these interphase areas play a dominant role in determining the unique dielectric properties of the nanocomposites. The permittivity usually increases, if polymers are filled with inorganic fillers of micrometer size by several tens wt%. It is because the fillers have higher permittivity by nature than unfilled polymers. Conversely, the permittivity is found to decrease in many cases, if polymers are filled with fillers of nanometer size by several wt% [8]. But increase values also available in nanocomposites. It is possibly due to any accidental inclusion of the imperfection of nanocomposites such as inhomogeneous dispersion and agglomeration of nanofillers that are technically difficult to avoid, impurities unintentionally mixed in during manufacturing processes, residual curing agents and diluting agents (dispersants) if used.

1.2 Problem Statement

As mentioned earlier, the use of nanofillers is promising to enhance dielectric properties such as improved partial discharge resistance, suppressed space charge formation and reduced treeing progression. Recent research claimed the enhancement of properties is attributed to the presence of large interphase area which is the interaction zone between the particles and the matrix. Many studies modelled the polymer with assumptions that all nanoparticles were dispersed homogeneously in nanocomposites. However, ensuring that particles are dispersed homogeneously distributed in the polymer matrix is still challengeable.

1.3 Objectives of the Research

The objectives of this research are:

(a) To model the electric field distribution in nanocomposites containing non-homogeneously dispersed nanofillers.

(b) To determine the effect of electric field distribution in relation to different nanofiller properties and their interphase.

(c) To propose the mechanisms leading to the changes in dielectric properties based on the model nanocomposite systems.

1.4 Scope of the Research

This project focuses on the effect of nanofillers and their interphase on the electric field distribution in polymer nanocomposites. The model of the electric field distribution in nanocomposites with the presence of nanofillers and their interphases was performed using the Finite Element Method Magnetics (FEMM) 4.2 software. In this project, the model was based on polymer (polyethylene) and spherical nanoparticle (silica) with assumed fixed permittivity values with nanoparticle distribution within nanocomposites is nonhomogeneous. Then, in order to determine the effects on electric field distribution in nanocomposite systems, changes in the models were determined by varying nanoparticles size, the interphase thickness, the permittivity values within interphase and position of nanoparticles.

1.5 Timeline of the Project

Table 1.2 and 1.3 shows the planned timeline for the project.

Table 1.2 Planned timeline for Project 1

No.	Project 1 Schedule	SEMESTER 1														
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	Confirmation Letter															
2	Literature Review															
3	Project Synopsis Preparation															
4	Project Synopsis Submission															
5	FEMM-4.2 software familiarization															
6	Seminar Material Preparation															
7	Submission of Seminar Material															
8	Seminar Presentation															
9	Report Preparation and Submission															

Table 1.3 Planned timeline for Project 2

No.	Project 2 Schedule	SEMESTER 2														
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	Literature Review															
2	Modelling and Simulation on nanocomposites with the presence of nanofillers: a. Varying the interphase permittivity. b. Varying the size of nanoparticles and interphase. c. Varying the position and distance between adjacent of particles.															
3	Analyzed simulation results															
4	Discussion and conclusion															
5	Preparations for final seminar															
6	Thesis preparation and editing															
7	Thesis submission															

1.6 Thesis Structure and Organization

Chapter 2 is about literature review. It provides the background theories of previous work concerning on concept of nanocomposites, modelling and simulation, polymer structure and properties, nanoparticles and interphase region and electric field distribution analysis.

Chapter 3 contains research methodology that explains in detail on how to achieve the objectives of this project which include methodology on modelling and simulation polymer nanocomposites system using FEMM 4.2 simulator. The parameters of model, including the size of particle, permittivity value, interphase diameter and type of particle dispersion are explained and presented in this chapter.

The simulation results taken based on the models in Chapter 3 and data analyses are covered in Chapter 4. This chapter starts with a basic polymer model without particles, then with single microparticle and single nanoparticle with and without interphase. To investigate the effects of nanoparticle dispersion in electric fields distribution, there are four different particle dispersion cases that been simulated through FEMM 4.2 based on 110 nanosilica particles. The first case is homogenous and the other three cases are non-homogenous namely as centralised dispersion and 2 cases of random dispersion. Other than particles dispersion factor, this chapter also discussed the effects of nanoparticles size, the interphase thickness and permittivity value within interphase to electric field distribution.

Lastly, Chapter 5 summarizes all the results and discussions on the electric distribution in polymer nanocomposites. The outlook and aim of this work are again highlighted with recommendation for future research work.

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