

DETECTION OF AMMONIA IN NEAR INFRARED REGION CONSIDERING  
THE EFFECT OF CROSS SENSITIVITY

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A thesis submitted in fulfilment of the  
requirements for the award of the degree of  
Master of Engineering (Electrical)

Faculty of Electrical Engineering  
Universiti Teknologi Malaysia

NOVEMBER 2013

*Dedicated and thankful appreciation to my beloved parents, brothers, sisters,  
friends and lecturers for their support, encouragement and understandings.*

## **ACKNOWLEDGEMENT**

First and foremost, praise is upon Allah S.W.T, the Almighty for giving me the opportunity and strength to accomplish this project and also the thesis.

My gratitude goes to my supervisor, Assoc. Prof. Dr. Sevia Mahdaliza Idrus and my co-supervisor Assoc. Prof. Dr Mohamad Haniff Ibrahim for his precious assistance and guidance given throughout the progress of this project.

My sincere appreciation is extended to the funders, Ministry of Higher Education and Universiti Teknologi Malaysia for the financial support throughout this research

My appreciation also goes to my beloved father, mother and siblings for motivating and supporting me throughout this experience. Thanks for their encouragement, love and emotional supports that they had given to me.

Finally, I would like to express my heartfelt gratitude to Lightwave Communication Research Group members and to all my professors and all also those whoever has helped me either directly or indirectly in the completion of my master project and thesis.

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## ABSTRACT

Ammonia gases have their own advantages and disadvantages; however it is important to monitor ammonia emission to avoid hazardous level. Ultraviolet or broadband Infrared absorption, and Photothermal Deflection prevent the species-conversion, time delay, and adsorption problems associated with traditional sampling systems, but often use expensive, bulky or delicate radiation sources that are not suitable for commercialisation. In gas detection, cross sensitivity is one of the constraints since the air consists of a variety of gases. A few techniques were introduced such as using gas separation techniques or ratio calculation to overcome the problem. For ammonia gas sensing, it has been reported that the cross sensitivity with humidity is the main problem and this occurs in certain wavelength ranges. This is a strong indication that cross sensitivity for ammonia emission monitoring must be modelled. Choosing suitable wavelength of ammonia with minimal cross sensitivity effect can reduce the effect of cross sensitivity at infrared region. In this numerical prediction analysis, the optical transmission of ammonia was obtained through a model developed using a commercial simulator SpectralCalc-GATS, OptiSystem and Matlab. The developed model is then interfaced with the integrated sensor system model using OptiSystem for system performance and characterisation. The simulation shows that ammonia absorption cross section within 2200 nm to 2400 nm region has less cross sensitivity issues. It is not possible to discuss the cross sensitivity issue for every single atmospheric gas as there are too many gases in the atmosphere and the amount is small and subject to the surrounding environment. These simulations consider other gases such as CO<sub>2</sub> and H<sub>2</sub>O Proper cross sensitivity is able to be simulated and characterised through the sensor model developed through this research.

## ABSTRAK

Gas ammonia mempunyai kelebihan dan kekurangan yang tersendiri; walau bagaimanapun, pembebasan ammonia adalah penting untuk dipantau bagi mengelakkan daripada berlakunya pembebasan gas yang berbahaya. Ultraungu atau penyerapan jalur lebar Infrared, dan Pesongan Photothermal mengelakkan spesis penukaran, masa tunda, dan penyerapan masalah yang berkaitan dengan sistem pensampelan tradisional, mahal, sumber radiasi yang besar atau halus yang tidak sesuai untuk dikomersialkan. Beberapa teknik telah diperkenalkan seperti menggunakan teknik pemisahan gas atau pengiraan nisbah untuk mengatasi masalah ini. Bagi pengesan gas ammonia, ia telah dilaporkan bahawa sensitiviti rentas dengan kelembapan adalah masalah utama dan berlaku dalam julat panjang gelombang tertentu. Ini menunjukkan bahawa sensitiviti silang untuk pemantauan pelepasan ammonia mesti di modelkan. Pemilihan panjang gelombang ammonia yang sesuai boleh mengurangkan masalah sensitiviti silang pada kawasan infrared. Dalam analisis berangka ini, penghantaran optik ammonia telah diperolehi melalui model yang dibangunkan dengan menggunakan simulator komersial *SpectralCalc-GATS*, *OptiSystem* dan Matlab. Model yang dibangunkan kemudian bersepada dengan sistem model menggunakan *OptiSystem* untuk prestasi sistem dan pencirian. Simulasi menunjukkan bahawa ammonia penyerapan keratan rentas dalam 2200 nm untuk 2400 nm menghadapi kurang masalah sensitiviti silang. Ianyad tidak mungkin untuk membincangkan isu sensitiviti rentas untuk setiap gas atmosfera tunggal kerana terdapat terlalu banyak gas di dalam atmosfera dan jumlah tersebut adalah kecil dan tertakluk kepada alam sekitar. Simulasi ini mempertimbangkan gas lain seperti CO<sub>2</sub> dan H<sub>2</sub>O. Melalui model sensor yang dibangunkan melalui penyelidikan ini, kepekaan sensitiviti silang mampu untuk disimulasikan dan dicirikan.

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**LIST OF ABBREVIATIONS**

NH <sub>3</sub>	-	Ammonia
PON	-	Carbon Dioxide
CO <sub>2</sub>	-	Water
H <sub>2</sub> O	-	Part Per Million
Ppm	-	Infrared
IR	-	Part Per Billion
Ppb	-	Part Per Billion
PTFE	-	Polytetrafluoroethylene
MOS	-	Metal Oxide Semiconductor
ZnO	-	Zinc Oxide
SO <sub>2</sub>	-	Sulfur dioxide
CO	-	Central Office
UV	-	Ultraviolet
NMR	-	Nuclear Magnetic Resonance

**LIST OF SYMBOLS**

$^{\circ}C$	-	Celsius
$s$	-	Second
$cm$	-	Centimeter
$E_p$	-	Energy of the Photon
$h$	-	Planck's Constant
$\Lambda$	-	Wavelength
$\nu_p$	-	Frequency of the Photon
$c$	-	Speed of Light in a Vacuum
$N_A$	-	Avogadro's Constant
$T$	-	Temperature
$A$	-	Absorbance
$P$	-	Pressure
$k$		Boltzmann constant

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# **CHAPTER 1**

## **INTRODUCTION**

### **1.1 Background**

For a long time, there has been a lot of interest to study the relationship between the human activities and the changes in the environment. The main reason for this is that various human activities have produced a lot of emissions in term of gases and other materials that pollute the environment [1]. Well-known phenomena such as global climatic change, photochemical smog formation, acid rain, stratospheric ozone depletion and forest decline are strongly related to various human activities in various sectors such as industry, agriculture, domestic, transportation, and urbanization just to name a few [2].

Ammonia has been widely used in the production of explosives, fertilizers, and as an industrial coolant. The excess presence of ammonia in the atmosphere may create potential hazards to human being and ecosystems. Inhalation of only a small dose of ammonia vapor may cause acute poisoning to people. Threshold limit of ammonia concentration in air is only 25 ppm for human beings. In addition, the fast, realtime quantification of atmospheric ammonia concentration is particularly

important for environmental chemistry because ammonia is the most abundant alkaline component in the atmosphere.

## **1.2 Problem Statement**

Most people are exposed to ammonia from inhalation of the gas or vapours. Since ammonia exists naturally and is also present in cleaning products, exposure may occur from these sources. The widespread use of ammonia on farms and in industrial and commercial locations also means that exposure can occur from an accidental release or from a deliberate terrorist attack. Many optical techniques also employ derivative or FM spectroscopy to increase sensitivity, but require calibration gases to provide reference signals and have complicated lineshapes due to the overlapping of multiple NH<sub>3</sub> absorption lines .The simulation of ammonia is never been done of any researcher, this simulation will help the researcher to choose the right wavelength where that we can reduce the effect of cross sensitivity. Choosing the right wavelength can help the researcher to build more accurate sensor. Hence, this is a strong indication that sensor that not influence by cross sensitivity for ammonia emission monitoring must be model. This simulation is important to give the overview of the system which is capable to detecting of ammonia emission.

## **1.3 Objectives**

The objectives of this study are:

1. To design an optical fiber based sensor system that would be capable of detecting ammonia gas emission.

2. To propose the suitable wavelength range of ammonia sensing operation in order to reduce the effect of cross sensitivity.

#### **1.4 Scopes of Project**

The foremost part of this research is to conduct a comprehensive theoretical analysis of the developed sensor system. The analysis is conducted by taking into consideration the transmission spectra of the sensor components e.g. to simulate the expected sensor output in terms of the optical transmission and also absorption for various concentrations of the target gas. After completion of the theoretical analysis, the developed sensor system will be modelling. The sensor system will be used to detect the emission of ammonia. LED laser array will be used as source and will transmit the light to the gas cell. The gas cell will be done at Matlab and the data from SpectralCalc will be include inside Matlab. The result will be shown at optisystem.

#### **1.5 Research Methodology**

The flow for this research study is briefly shown in the flow chart in Figure 1.1.

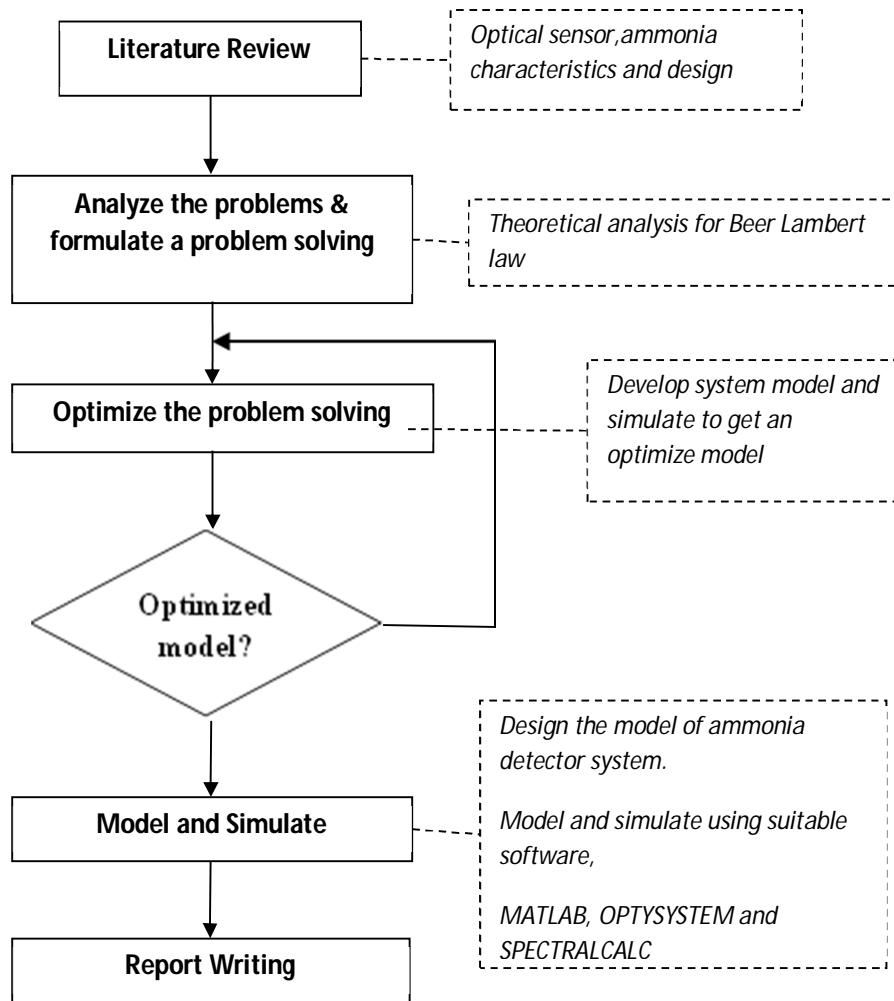


Figure. 1.1: Project flow chart

The project begins with the literature study and understanding of the basic of ammonia. Then, the theoretical of beer lambert law must be understand before proceed to the main problem of this project. Next, develop system model using spectralcalc which is all possible ammonia region has been categorized. The suitable wavenumber had been study to use the data from spectralcalc to overlap with optisystem and matlab.

Parameters in the system is studied and considered. Then, simulation of ammonia system is designed.

Next, the ammonia system design is modeled and simulated using OptiSystem and Matlab.

Finally, report writing and publications are done.

## **1.6 Thesis Outline**

This thesis consists of five chapters and it is organized as follows:

Chapter 1 discussed on the research background, problem statement, objective, scope of project, research methodology, and the outline of the thesis.

Chapter 2 is a introduction of ammonia, characteristic of ammonia and review of current ammonia sensors that have been reported to date in the literature. Some of the sensors have been commercialized and are presently used in many areas and applications. A brief explanation of various sensor configurations is presented and theoretical assessment and suitability of each sensor is carried out before the process of designing and developing a new sensor that can detect ammonia in environment commences.

Chapter 3 cover the background and the description of each procedure of optysystem, Matlab and Spectralcalc

Chapter 4 mainly discuss about the result from simulation of Matlab, Optysystem and SpectralCalc.

Chapter 5 includes the conclusion and recommendation of the thesis.

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