CHANNEL MODELING OF MULTILAYER DIFFUSION-BASED MOLECULAR NANO COMMUNICATION SYSTEM

SAIZALMURSIDI BIN MD MUSTAM

UNIVERSITI TEKNOLOGI MALAYSIA
CHANNEL MODELING OF MULTILAYER DIFFUSION-BASED MOLECULAR NANO COMMUNICATION SYSTEM

SAIZALMURSIDI BIN MD MUSTAM

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

Faculty of Electrical Engineering
Universiti Teknologi Malaysia

AUGUST 2016
To my beloved father, mother, wife and sons for their endless love, encouragement and support.
ACKNOWLEDGEMENT

I would like to express my deepest gratitude to my supervisor, Associate Professor Dr. Sharifah Kamilah binti Syed Yusof for giving me an opportunity to work under her guidance, and for her trust, support and encouragement throughout the entire duration of my Ph.D study. I am also thankful for her unbounded energy and passion, which helped me to steadily advance towards the successful completion of this thesis.

I would also like to extend my appreciation to all staffs of the Faculty of Electrical Engineering, Universiti Teknologi Malaysia (UTM) Skudai, who have involved directly or indirectly throughout the period of my Ph.D study. In particular, I would like to sincerely thanks Professor Dr. Norshiela binti Fisal for her invaluable comments, advises and motivation which have helped me to achieve a solid research path towards this thesis. To all my colleagues and fellow researchers in the UTM-MIMOS Telecommunication Technology Research Group, thank you for the unique atmosphere, constant support and true friendship we have had during my research period.

I would also like to thank the Ministry of Higher Education, Malaysia, and the University Tun Hussein Onn Malaysia (UTHM) for the financial support provided in the form of a doctoral scholarship and monthly allowances.

Special thanks are due to my parents, Md Mustam bin Marzuki and Sa’emah binti Ngadi, my wife Fazlina binti Yunus and my sons Muhammad Sadiq and Muhammad Faqih, for their understanding, patience, encouragement, support and love.

Last but not least, I would like to thank the developers of the utmthesis \LaTeX\ project for making the thesis writing process a lot easier for me. Thanks to them, I could focus on the content of the thesis, and not waste time with formatting issues. Those guys are awesome.
ABSTRACT

In nanoscale communication, diffusion-based molecular communication (DBMC) in which information is encoded into molecule patterns by a transmitter nanomachine, has emerged as a promising communication system, particularly for biomedical and healthcare applications. Although, numerous studies have been conducted to evaluate and analyze DBMC systems, investigation on DBMC system through a multilayer channel has received less attention. The aims of this research are to mathematically model a closed-form expression of mean molecular concentration over multilayer DBMC channel, to formulate channel characteristics, and to conduct performance evaluation of multilayer DBMC channel. In the mathematical model, the propagation of molecules over an \( n \)-layer channel is assumed to follow the Brownian motion and subjected to Fick’s law of diffusion. The partial differential equation (PDE) of the time rate change of molecular concentration is obtained by modeling the \( n \)-layer channel as an \( n \)-resistor in series and considering the conservation law of molecules. Fourier transform and Laplace transform were used to obtain the solution for the PDE, which represents the mean molecular concentration at a receiver nanomachine. In the formulation, channel characteristics such as impulse response, time delay, attenuation or the maximum peak, delay spread and capacity were analytically obtained from the mean molecular concentration. In this stage, the multilayer channel is considered as a linear and deterministic channel. For the performance evaluation, the air-water-blood plasma medium representing the simplified multilayer diffusion model in the respiratory system was chosen. It was found that both analytical and simulation results of mean molecular concentration using Matlab and N3Sim were in good agreement. In addition, the findings showed that the higher the average diffusion coefficient resulted in a smaller dispersion of channel impulse response, and shortened the channel delay spread as well as time delay. However, the channel attenuation remains unchanged. In the performance evaluation, an increase of 100% in the transmission distance increased the time delay by 300% but decreased the maximum peak of molecular concentration by 87.5%. A high channel capacity can be achieved with wide transmission bandwidth, short transmission distance, and high average transmitted power. These findings can be used as a guide in the development and fabrication of future artificial nanocommunication and nanonetwork systems involving multilayer transmission medium. Implication of this study is that modeling and analyzing of multilayer DBMC channel are important to support biomedical applications as diffusion can occur through a multilayer structure inside the human body.
ABSTRAK

# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>CHAPTER</th>
<th>TITLE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>DECLARATION</td>
<td></td>
<td>ii</td>
</tr>
<tr>
<td>DEDICATION</td>
<td></td>
<td>iii</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENT</td>
<td></td>
<td>iv</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td></td>
<td>v</td>
</tr>
<tr>
<td>ABSTRAK</td>
<td></td>
<td>vi</td>
</tr>
<tr>
<td>TABLE OF CONTENTS</td>
<td></td>
<td>vii</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td></td>
<td>xi</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td></td>
<td>xii</td>
</tr>
<tr>
<td>LIST OF ABBREVIATIONS</td>
<td></td>
<td>xvi</td>
</tr>
<tr>
<td>LIST OF SYMBOLS</td>
<td></td>
<td>xvii</td>
</tr>
<tr>
<td>LIST OF APPENDICES</td>
<td></td>
<td>xxi</td>
</tr>
</tbody>
</table>

1 INTRODUCTION 1

1.1 Background 1
1.2 Problem Statement 3
1.3 Research Objectives 4
1.4 Research Scopes 4
1.5 Research Contributions 6
1.6 Significance of Research 8
1.7 Thesis Outline 8

2 LITERATURE REVIEW 10

2.1 Introduction 10
2.2 Nanocommunication and Nanonetworks 11
  2.2.1 Nano-electromagnetic Communication 13
  2.2.2 Molecular Communication 13
2.3 Overview of Diffusion-Based Molecular Communication (DBMC) System 15
2.3.1 Encoding and Transmission of Information Molecules 15
2.3.2 Propagation or Diffusion of Information Molecules 16
2.3.3 Reception and Decoding of Information Molecules 18

2.4 Related Research Works 18
2.4.1 The DBMC Channel Modeling 18
2.4.2 Multilayer Diffusion 21

2.5 Context of the Research 22

2.6 Summary 22

3 RESEARCH METHODOLOGY 24
3.1 Introduction 24
3.2 Research Procedures 25
3.2.1 Mathematical Modeling of Multilayer DBMC Channel 27
3.2.1.1 Derivation of mean molecular concentration at RN 28
3.2.1.2 Development of Simulation Model using N3Sim Simulator 29
3.2.1.3 Formulation of Multilayer DBMC Channel Impulse Response, Time Delay, Attenuation and Delay Spread 30
3.2.1.4 Derivation of Multilayer DBMC Channel Capacity 31
3.2.2 Performance Evaluation of Multilayer DBMC Channel 31
3.2.2.1 Performance Metrics 31
3.2.2.2 A Multilayer Medium Under Study 32

3.3 Analytical and Numerical Analysis Tools 34

3.4 Summary 34

4 MATHEMATICAL MODELING OF MULTILAYER DBMC CHANNEL 35
4.1 Introduction 35
4.2 Multilayer DBMC Channel Modeling 36
4.2.1 Mean Molecular Concentration over $n$–Layer Channel 37
4.2.2 Mean Number of Received Molecules 43
4.3 Formulation of Multilayer DBMC Channel Characteristics 44
4.3.1 Channel Impulse Response 44
4.3.2 Channel Time Delay 44
4.3.3 Channel Attenuation 45
4.3.4 Channel Delay Spread 46
  4.3.4.1 Delay Spread of Impulse Transmission over Multilayer DBMC Channel 46
  4.3.4.2 Spreading of a Square Pulse Transmission over Multilayer DBMC Channel 49
4.3.5 Channel Capacity 53
  4.3.5.1 The Fick’s Diffusion Mutual Information 54
  4.3.5.2 The Capacity of Multilayer DBMC Channel 56
4.4 Summary 57

5 PERFORMANCE ANALYSIS OF MULTILAYER DBMC CHANNEL 58
5.1 Introduction 58
5.2 Channel Impulse Response, $h(r, t)$ 61
5.3 Mean Molecular Concentration, $c(r, t)$ 63
5.4 Mean Number of Received Molecules, $s(r, t)$ 65
  5.4.1 Effects of Layer Fraction, $f_i$ on the Maximum Mean Number of Received Molecules, $s(r, t)_{max}$ and Time Delay, $t_d$ 66
  5.4.2 Effects of Transmission Distance, $r$ on the Maximum Mean Number of Received Molecules, $s(r, t)_{max}$ and Time Delay, $t_d$ 68
  5.4.3 Effects of Total Number of Transmitted Molecules, $Q_0$ on the Maximum Mean Number of Received Molecules, $s(r, t)_{max}$ and Time Delay, $t_d$ 73
5.5 Analysis of Delay Spread in Multilayer DBMC Channel

5.5.1 Effects of Multilayer Channel on the Channel Delay Spread, $\tau_h$ 75

5.5.2 Effects of Transmission Distance, $r$ on the Channel Delay Spread, $\tau_h$ 78

5.5.3 Effects of Total Number of Transmitted Molecules, $Q_0$ on the Channel Delay Spread, $\tau_h$ 80

5.5.4 Effects of Data Rate of Transmitted Bit, $R_b = 1/T_b$ on the Pulse Spreading 82

5.6 Analysis of Capacity in Multilayer DBMC Channel 83

5.6.1 Transfer Function Fourier Transform of Channel Impulse Response, $h(r, f)$ 84

5.6.2 Capacity, $C$ versus Bandwidth, $W$ for Different Values of Transmission Distance, $r$ 85

5.6.3 Capacity, $C$ versus Transmission Distance, $r$ for Different Values of Bandwidth, $W$ 86

5.6.4 Capacity, $C$ versus Transmission Distance, $r$ for Different Values of Layer Fraction, $f_i$ 88

5.6.5 Capacity, $C$ versus Bandwidth, $W$ for Different Values of the Average Power Transmission, $P^\text{H}$ 89

5.7 Summary 90

6 CONCLUSIONS 91

6.1 Conclusions 91

6.2 Recommendations for Future Work 94

REFERENCES 95

Appendices A – I 104 – 137
# LIST OF TABLES

<table>
<thead>
<tr>
<th>TABLE NO.</th>
<th>TITLE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Nano-electromagnetic versus molecular communications</td>
<td>13</td>
</tr>
<tr>
<td>2.2</td>
<td>Summary of related works on point-to-point DBMC channel model</td>
<td>23</td>
</tr>
<tr>
<td>5.1</td>
<td>Simulation parameters</td>
<td>59</td>
</tr>
<tr>
<td>5.2</td>
<td>Effects of doubling and halving of $r = 45 \mu m$ on $s(r,t)_{max}$ and $t_d$</td>
<td>69</td>
</tr>
<tr>
<td>5.3</td>
<td>Channel delay spread, $\tau_h$ and pulse spreading of a square pulse transmission with $T_b = 5 \text{ s}$</td>
<td>77</td>
</tr>
<tr>
<td>5.4</td>
<td>Numerical analysis parameters</td>
<td>83</td>
</tr>
</tbody>
</table>
LIST OF FIGURES

<table>
<thead>
<tr>
<th>FIGURE NO.</th>
<th>TITLE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>An overview of nanonetworks: (a) nano-electromagnetic communication, and (b) molecular communication</td>
<td>12</td>
</tr>
<tr>
<td>2.2</td>
<td>Molecular communication with (a) active transport, and (b) passive transport by diffusion</td>
<td>14</td>
</tr>
<tr>
<td>2.3</td>
<td>Diffusion-based molecular communication (DBMC) system</td>
<td>15</td>
</tr>
<tr>
<td>2.4</td>
<td>Multilayer structures: (a) an alveolar-blood capillary barrier, and (b) the stomach-blood barrier</td>
<td>21</td>
</tr>
<tr>
<td>3.1</td>
<td>Flowchart of the research activities</td>
<td>26</td>
</tr>
<tr>
<td>3.2</td>
<td>Block diagram of the research framework</td>
<td>27</td>
</tr>
<tr>
<td>3.3</td>
<td>A multilayer diffusion-based molecular communication (DBMC) system</td>
<td>28</td>
</tr>
<tr>
<td>3.4</td>
<td>Flowchart of simulation steps using N3Sim simulator</td>
<td>29</td>
</tr>
<tr>
<td>3.5</td>
<td>Multilayer DBMC channel over the air-water-blood plasma medium (a) a physical system, and (b) the simplified representation</td>
<td>33</td>
</tr>
<tr>
<td>4.1</td>
<td>(a) Ohm’s circuit law and (b) the equivalent relationship between the radial diffusive flux and the concentration difference of molecules</td>
<td>39</td>
</tr>
<tr>
<td>4.2</td>
<td>Multilayer diffusion: (a) a thin interlayer between n thick different mediums and (b) its equivalent circuit</td>
<td>40</td>
</tr>
<tr>
<td>4.3</td>
<td>(a) Impulse transmission sequence with symbol interval, $T_s$ and, (b) the response of mean molecular concentration due to impulsive transmission</td>
<td>47</td>
</tr>
<tr>
<td>4.4</td>
<td>(a) A square pulse molecules transmission with pulse duration, $T_b$ and average amplitude of $Q_{ave}$ and, (b) output response of mean molecular concentration due to a square pulse molecules transmission</td>
<td>49</td>
</tr>
<tr>
<td>4.5</td>
<td>Information-theoretic diagram of multilayer DBMC system</td>
<td>53</td>
</tr>
<tr>
<td>4.6</td>
<td>Venn diagram of the mutual information between the input signal $X$ and output signal $Y$</td>
<td>54</td>
</tr>
</tbody>
</table>
5.1 Multilayer diffusion: (a) an alveolar-blood barrier and, (b) the simplified multilayer representation

5.2 Channel impulse responses for air, water, blood plasma, water-blood plasma and air-water-blood plasma mediums with a separation distance of $r = 45 \, \mu m$

5.3 Mean molecular concentration at the RN location, for a pulse transmission of $5 \times 10^5$ molecules through single layer medium with diffusion coefficient, $D$ of $1 \, \text{nm}^2/\text{ns}$ (ionic calcium in the cytoplasm) and transmission distance of $3 \, \mu m$

5.4 Analytical and simulation results of mean molecular concentration at the RN sensing volume, for the transmission of $2 \times 10^5$ molecules through water-blood plasma and air-water-blood plasma mediums with the transmission distance of $45 \, \mu m$

5.5 Analytical and simulation results of mean number of received molecules at the RN sensing volume, for the transmission of $2 \times 10^5$ molecules through water-blood plasma and air-water-blood plasma propagation mediums with the transmission distance of $45 \, \mu m$

5.6 Mean number of received molecules at the RN ($r = 45 \, \mu m$) over the water ($D_{\text{water}}$), blood plasma ($D_{\text{blood}}$), and water-blood plasma mediums with different fractions of layer thicknesses ($D_{av,1}$, $D_{av,2}$, and $D_{av,3}$)

5.7 Mean number of received molecules at the RN ($r = 45 \, \mu m$) over the air ($D_{\text{air}}$), blood plasma ($D_{\text{blood}}$), and air-blood plasma mediums with different fractions of layer thicknesses ($D_{av,1}$, $D_{av,2}$, and $D_{av,3}$)

5.8 Mean number of received molecules at the RN over the water-blood plasma medium ($f_1 = f_2 = 0.5$) when (a) doubling the TN–RN distance from $45 \, \mu m$ to $90 \, \mu m$ and, (b) halving the TN–RN distance from $45 \, \mu m$ to $22.5 \, \mu m$

5.9 Mean number of received molecules at the RN over the air-blood plasma medium ($f_1 = f_2 = 0.5$) when (a) doubling the TN–RN distance from $45 \, \mu m$ to $90 \, \mu m$ and, (b) halving the TN–RN distance from $45 \, \mu m$ to $22.5 \, \mu m$

5.10 Mean number of received molecules at the RN over the air-water-blood plasma medium ($f_1 = f_2 = f_3 = 1/3$) when (a) doubling the TN–RN distance from $45 \, \mu m$ to $90 \, \mu m$ and, (b) halving the TN–RN distance from $45 \, \mu m$ to $22.5 \, \mu m$
5.11 Mean number of received molecules at the RN over the water-blood plasma medium \((f_1 = f_2 = 0.5)\) for 45 \(\mu\)m of the TN–RN distance when varying the number of transmitted molecules from \(2 \times 10^5\) to \(4 \times 10^5\) and \(8 \times 10^5\) molecules.

5.12 Mean number of received molecules at the RN over the air-blood plasma medium \((f_1 = f_2 = 0.5)\) for 45 \(\mu\)m of the TN–RN distance when varying the number of transmitted molecules from \(2 \times 10^5\) to \(4 \times 10^5\) and \(8 \times 10^5\) molecules.

5.13 Mean number of received molecules at the RN over the air-water-blood plasma medium \((f_1 = f_2 = f_3 = 1/3)\) for 45 \(\mu\)m of the TN–RN distance when varying the number of transmitted molecules from \(2 \times 10^5\) to \(4 \times 10^5\) and \(8 \times 10^5\) molecules.

5.14 Normalized mean molecular concentration at the RN for 45 \(\mu\)m of the TN–RN distance, over the air-water-blood plasma \((D_{av,1})\), air-air-blood plasma \((D_{av,2})\), and air-air-water plasma \((D_{av,3})\) mediums with layer fraction of \(f_1 = f_2 = f_3 = 1/3\) due to (a) an impulsive transmission of molecules, and (b) a square pulse transmission of molecules with \(T_b = 5\) s.

5.15 Normalized mean molecular concentration at the RN over the air-water-blood plasma medium with equal layer fraction \((f_1 = f_2 = f_3 = 1/3)\) when increasing the TN–RN distance from 22.5 \(\mu\)m to 30 \(\mu\)m and 45 \(\mu\)m due to (a) an impulsive transmission and, (b) a square pulse transmission with \(T_b = 5\) s.

5.16 Normalized mean molecular concentration at the RN for 45 \(\mu\)m of the TN–RN distance, over the air-water-blood plasma medium with equal layer fraction \((f_1 = f_2 = f_3 = 1/3)\) when increasing the number or transmitted molecules from \(2 \times 10^5\) to \(4 \times 10^5\) and \(8 \times 10^5\) due to (a) an impulsive transmission and, (b) a square pulse transmission with \(T_b = 5\) s.

5.17 Normalized mean molecular concentration at the RN for 45 \(\mu\)m of the TN–RN distance, over the air-water-blood plasma medium with equal layer fraction \((f_1 = f_2 = f_3 = 1/3)\) for a square pulse transmission with different pulse width, \(T_p\) of transmitted bit, \(T_b\).
5.18 Transfer function Fourier transform of channel impulse response over the air-water-blood plasma medium \((f_1 = f_2 = f_3 = 1/3)\) for 30 \(\mu\)m, 50 \(\mu\)m and 100 \(\mu\)m of the TN–RN distances

5.19 Capacity for various TN-RN distances as a function of bandwidth over the air-water-blood plasma medium \((f_1 = f_2 = f_3 = 1/3)\)

5.20 Capacity for various transmission bandwidths as a function of TN-RN distance over the air-water-blood plasma medium \((f_1 = f_2 = f_3 = 1/3)\)

5.21 Capacity for various layer fractions as a function of TN-RN distance over the air-water-blood plasma medium

5.22 Capacity for various average transmitted powers as a function of bandwidth over the air-water-blood plasma medium \((f_1 = f_2 = f_3 = 1/3)\)

A.1 Steady-state diffusion in one dimensional

B.1 Nonsteady-state diffusion in one dimensional
LIST OF ABBREVIATIONS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>BANs</td>
<td>Body Area Nanonetworks</td>
</tr>
<tr>
<td>dB</td>
<td>Decibel</td>
</tr>
<tr>
<td>C</td>
<td>Celcius</td>
</tr>
<tr>
<td>CSK</td>
<td>Concentration Shift Keying</td>
</tr>
<tr>
<td>DBMC</td>
<td>Diffusion-Based Molecular Communication</td>
</tr>
<tr>
<td>Hz</td>
<td>Hertz</td>
</tr>
<tr>
<td>IoBNT</td>
<td>Internet of Bio-Nano Things</td>
</tr>
<tr>
<td>ISI</td>
<td>Inter-Symbol Interference</td>
</tr>
<tr>
<td>MoSK</td>
<td>Molecule Shift Keying</td>
</tr>
<tr>
<td>OOK</td>
<td>On-Off Keying</td>
</tr>
<tr>
<td>ODE</td>
<td>Ordinary Differential Equation</td>
</tr>
<tr>
<td>PAM</td>
<td>Pulse Amplitude Modulation</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>RN</td>
<td>Receiver Nanomachine</td>
</tr>
<tr>
<td>TN</td>
<td>Transmitter Nanomachine</td>
</tr>
<tr>
<td>W</td>
<td>Watt</td>
</tr>
</tbody>
</table>
**LIST OF SYMBOLS**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta(r) )</td>
<td>Dirac’s delta function of the source location</td>
</tr>
<tr>
<td>( \delta(t) )</td>
<td>Dirac’s delta function of the source time</td>
</tr>
<tr>
<td>( \eta )</td>
<td>Dynamic viscosity of the fluidic medium</td>
</tr>
<tr>
<td>( \eta_{\text{air}} )</td>
<td>Dynamic viscosity of air</td>
</tr>
<tr>
<td>( \eta_{\text{water}} )</td>
<td>Dynamic viscosity of water</td>
</tr>
<tr>
<td>( \eta_{\text{blood}} )</td>
<td>Dynamic viscosity of blood plasma</td>
</tr>
<tr>
<td>( \tau_h )</td>
<td>Channel delay spread</td>
</tr>
<tr>
<td>( * )</td>
<td>Convolution operation</td>
</tr>
<tr>
<td>( v_0 - v_1 )</td>
<td>Voltage difference</td>
</tr>
<tr>
<td>( \nabla^2 )</td>
<td>Laplacian operator</td>
</tr>
<tr>
<td>( \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k} )</td>
<td>Three-dimensional gradient operator</td>
</tr>
<tr>
<td>( \frac{\partial c(r, t)}{\partial r} )</td>
<td>Molecular concentration gradient</td>
</tr>
<tr>
<td>( \frac{\partial c(r, t)}{\partial t} )</td>
<td>Time rate changes in molecular concentration</td>
</tr>
<tr>
<td>( \frac{dc(r, t)}{dt} )</td>
<td>First time derivative of mean molecular concentration</td>
</tr>
<tr>
<td>( \ell )</td>
<td>Total thickness of the propagation medium</td>
</tr>
<tr>
<td>( \ell/D )</td>
<td>Diffusive resistance of the medium</td>
</tr>
<tr>
<td>( \ell_i/D_i )</td>
<td>Diffusive resistance of the ( i )-layer</td>
</tr>
<tr>
<td>( \ell_i/\ell )</td>
<td>Fraction of the ( i )-layer</td>
</tr>
<tr>
<td>( \Delta c )</td>
<td>Concentration difference of molecules</td>
</tr>
<tr>
<td>( \Delta r )</td>
<td>Membrane thickness</td>
</tr>
<tr>
<td>( c(x, y, z, t) )</td>
<td>Mean molecular concentration in three dimensional space at time ( t )</td>
</tr>
<tr>
<td>( c(r, t) )</td>
<td>Mean molecular concentration</td>
</tr>
<tr>
<td>( c(r_0, t) )</td>
<td>Concentration of molecules at the location of TN</td>
</tr>
</tbody>
</table>
\( c(r_0 + \ell, t) \) - Concentration of molecules at the location of RN

\( c(r, t)_{\text{max}} \) - Channel attenuation, or maximum peak of mean molecular concentration

\( c_r(r, t) \) - First space derivative of mean molecular concentration

\( c_{rr}(r, t) \) - Second space derivative of mean molecular concentration

\( c_t(r, t) \) - First time derivative of mean molecular concentration

\( c_t(\omega, t) \) - First time derivative of Laplace transforms of \( C(\omega, t) \)

\( \text{erfc} \) - Complementary error function

\( f_i \) - Fraction of the \( i \)-layer

\( f_z(x) \) - Probability density function of all the possible transmitted signal \( X \)

\( h(r, f) \) - Transfer function Fourier transform of the channel impulse response

\( h(r, t) \) - Channel impulse response

\( i \) - An integer 1, 2, 3, ...

\( \text{inverfc} \) - Inverse operation of the complementary error function

\( k \) - Partition coefficient of membrane

\( k_B \) - Boltzmann constant

\( n \) - Number of layers

\( r \) - Transmission distance or TN-RN distance

\( r_m \) - Radius of molecules

\( r_s \) - Radius of receiver sensing volume

\( s(r, t) \) - Mean number of received molecules

\( t \) - Time

\( t_d \) - Time delay

\( A \) - Area

\( C \) - Channel capacity

\( D \) - Diffusion coefficient

\( D_{av} \) - Average diffusion coefficient

\( D_i \) - Diffusion coefficient of the \( i \)-layer

\( H(X) \) - Entropy per second of the transmitted signal \( X \)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H(Y)$</td>
<td>Entropy per second of the received signal $Y$</td>
</tr>
<tr>
<td>$H(\dot{Q})$</td>
<td>Entropy of the number of transmitted molecules per time sample of the time function signal $Q(t)$</td>
</tr>
<tr>
<td>$H(X,Y)$</td>
<td>Joint entropy per second of the transmitted signal $X$ and the received signal $Y$</td>
</tr>
<tr>
<td>$H(X</td>
<td>Y)$</td>
</tr>
<tr>
<td>$I$</td>
<td>Current</td>
</tr>
<tr>
<td>$I(X;Y)$</td>
<td>Mutual information</td>
</tr>
<tr>
<td>$J$</td>
<td>Flux or diffusion rate per unit area</td>
</tr>
<tr>
<td>$J(x,t)$</td>
<td>Net diffusion flux at $x$ and at time $t$</td>
</tr>
<tr>
<td>$J(x+\ell,t)$</td>
<td>Net diffusion flux at $x+\ell$ and at time $t$</td>
</tr>
<tr>
<td>$J(r,t)$</td>
<td>Net radial diffusion flux</td>
</tr>
<tr>
<td>$\vec{J}(x,y,z,t)$</td>
<td>Flux vector in three dimensional space at time $t$</td>
</tr>
<tr>
<td>$N(x,t)$</td>
<td>Molecules at position $x$ and time $t$</td>
</tr>
<tr>
<td>$N(x+\delta,t)$</td>
<td>Molecules at position $x+\delta$ and time $t$</td>
</tr>
<tr>
<td>$dN$</td>
<td>Net number of particles</td>
</tr>
<tr>
<td>$P$</td>
<td>Permeability coefficient</td>
</tr>
<tr>
<td>$\bar{P}_H$</td>
<td>Average thermodynamic power in molecules transmission</td>
</tr>
<tr>
<td>$Q$</td>
<td>Total number of transmitted molecules</td>
</tr>
<tr>
<td>$Q_0$</td>
<td>Total number of transmitted molecules</td>
</tr>
<tr>
<td>$Q_{ave}$</td>
<td>Average number of transmitted molecules</td>
</tr>
<tr>
<td>$Q(t)$</td>
<td>Time function of molecule transmission</td>
</tr>
<tr>
<td>$R$</td>
<td>Resistance</td>
</tr>
<tr>
<td>$R_b$</td>
<td>Data rate of transmitted bits</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
</tr>
<tr>
<td>$T_b$</td>
<td>Pulse bit duration</td>
</tr>
<tr>
<td>$T_s$</td>
<td>Symbol duration or interval</td>
</tr>
<tr>
<td>$V$</td>
<td>Receiver sensing volume</td>
</tr>
<tr>
<td>$dV$</td>
<td>Differential volume</td>
</tr>
<tr>
<td>$W$</td>
<td>Bandwidth of the transmitted signal</td>
</tr>
</tbody>
</table>
$X$ - Transmitted or input signal

$Y$ - Received or output signal

$C(\omega, t)$ - Fourier transforms of $c(r, t)$

$F(\omega)$ - Fourier transforms of $\delta(r)$

$\overline{C}(\omega, s)$ - Laplace transforms of $C(\omega, t)$

$\overline{F}(s)$ - Laplace transforms of $\delta(t)$
# LIST OF APPENDICES

<table>
<thead>
<tr>
<th>APPENDIX</th>
<th>TITLE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>The Fick’s First Law of Diffusion</td>
<td>104</td>
</tr>
<tr>
<td>B</td>
<td>The Fick’s Second Law of Diffusion</td>
<td>107</td>
</tr>
<tr>
<td>C</td>
<td>Solution of Diffusion Equation for an Impulsive Molecules Transmission</td>
<td>110</td>
</tr>
<tr>
<td>D</td>
<td>Solution of Diffusion Equation for a Time-Function Molecules Transmission</td>
<td>115</td>
</tr>
<tr>
<td>E</td>
<td>Solution of Multilayer Diffusion Equation for an Impulsive Molecules Transmission</td>
<td>120</td>
</tr>
<tr>
<td>F</td>
<td>Solution of Multilayer Diffusion Equation for a Time-Function Molecules Transmission</td>
<td>126</td>
</tr>
<tr>
<td>G</td>
<td>The Transfer Function Fourier Transform of Channel Impulse Response</td>
<td>132</td>
</tr>
<tr>
<td>H</td>
<td>Conditional Entropy per Second $H(X \mid Y)$ of the Transmitted Signal $X$ Given the Mean Molecular Concentration $Y$</td>
<td>136</td>
</tr>
<tr>
<td>I</td>
<td>List of Publications</td>
<td>137</td>
</tr>
</tbody>
</table>
CHAPTER 1

INTRODUCTION

1.1 Background

Rapid development in nanotechnology has motivated nanocommunication and nanonetworks of large numbers of nanoscale devices or nanomachines. Nanocommunication is a new research area where a communication process occurs between nanomachines. In a nanonetwork, a group of nanomachines is interconnected among them and expected to share information and coordinate activities to perform a specific task. With nanonetworks, the limited capabilities of a single nanomachine, such as only for computation, sensing, or actuation, can be expanded for executing more complex tasks and a wide range of applications. Interaction among networked nanomachines will allow the implementation of collaborative and synchronous tasks such as in-body drug delivery, disease treatments, and monitoring and controlling of environmental pollution [1].

Generally, nanocommunication can be realized through four different mechanisms, which are nanomechanical communication through mechanical contact, acoustic communication by using acoustic energy or pressure variations, nano-electromagnetic communication based on the modulation of terahertz electromagnetic waves, and molecular communication via transmission and reception of encoded information molecules [1]. However, both nano-electromagnetic communication and molecular communication have been envisioned as the two main options for wireless nanocommunication and nanonetworks [2]. Due to a small-scale, bio-compatible with the biological environment and energy efficiency of a molecular transceiver, molecular communication offers the most promising approaches for nanocommunication and nanonetworks among biological nanomachines as well as with the existing biological system [1, 3–6]. Another reason is that molecular communication can be approached through the observation of existing natural phenomena in biology [2, 7].
In the past decade, research activities have shown significant interests in the area of molecular communication to realize nanocommunication and nanonetworks. Numerous research efforts can be found in the literature to investigate the various models of molecular communication. Some of the proposed models are random walk [8,9], flow based or random walk with drift [10–12], diffusion based [2,3,12–15], diffusion-reaction based [16], walkway or active transport based [8, 17, 18] and collision based [19]. The performances of the proposed models are then analyzed in terms of channel capacity [9, 10], modulation schemes [9], normalized gain and delay [3], probability of reaching a receiver [17], transmission rate [11,12,15,17,18], mutual information [10,11], noise [13], throughput and efficiency [14], signal attenuation and amplification [16], collision rate [19], and communication range [15].

Among the proposed channel models, molecular communication by diffusion or diffusion-based molecular communication (DBMC) with and without drift has been the focus of interest in the research community [20]. The DBMC channel model is chosen as it represents the most basic and widespread molecular communication architecture found in nature [21, 22]. The concept of congestion in the DBMC channel for drug delivery near the targeted or disease area is introduced in [20]. A drug delivery system model using the DBMC with drift for drug transportation over bloodstream to only unhealthy parts inside the body can be found in [23]. Recently, the concept of body area nanonetworks (BANs) with DBMC for healthcare applications has been introduced in [5]. Furthermore, the concept of the Internet of Bio-Nano Things (IoBNT), involving the DBMC model for intra-body communication can be found in [24]. It is expected that from the proposed IoBNT, a healthcare provider can retrieve certain intra-body status parameters, such as glucose, sodium, and cholesterol levels, and the presence of unwanted agent through bio-nano things inside the body by using the Internet connection. The term bio-nano things can be referred to any type of nanosystems including liposomes [25–27], dendrimers [28], metallic nanoparticles [29], polymeric nanoparticles [30], carbon nanotubes [31] and nanowires [32, 33].

The current developments of nanotechnology in nanomedicine, tissue engineering, nanorobots, bio-sensor, bio-marker, and implant technologies have provided the possibilities of an intelligent system for an early disease detection and spontaneous targeted drug delivery in the treatment of human diseases in the near future. In these intelligent systems, a group of bio-nanomachines embedded in the human body or implanted under the skin are expected to communicate and cooperatively share information using molecular signals among each other or with the surrounding cells to perform a specific function such as synthesis the human health
condition, identifying the targeted drug delivery locations, and automatically control the amount and time of drug release. Moreover, the molecules of the drug are expected to be able to diffuse across a multilayer barrier or multiple environments towards the bloodstream as well as to the other parts inside the body or the infected area. Thus, a better understanding of how the drug’s molecules diffusing over the body and its concentration over time are utmost important for an effective disease treatment with an optimum amount of drugs.

1.2 Problem Statement

In nanoscale communication, the DBMC has emerged as one of the most promising communication models, particularly for health monitoring and drug delivery applications. In the DBMC, a transmitter nanomachine (TN) translates a message into encoded molecules and transmits them to a propagation medium or channel by opening a molecular gate. The transmitted molecules are then propagated from the TN to a receiver nanomachine (RN) over the channel by a diffusion process via Brownian motion. The RN captures the encoded molecules propagating in the channel and finally decodes the captured molecules.

Although, numerous studies have been conducted to evaluate and analyze DBMC system, investigation on DBMC through a multilayer channel due to variations in the medium properties or medium temperature has had less attention. The propagation of molecules over various mediums and environments or more complex medium, such as intracellular environment and the human body needs to be considered [4]. In practice, the diffusion of molecules can occur over the several layers in the human body, for example, diffusion of oxygen and carbon dioxide over the alveolar-blood barrier in the respiratory system [34], diffusion of digested particles, nutrients or medicine across the stomach-blood barrier during the absorption process, and diffusion of water, oxygen, carbon dioxide and lipid-soluble molecules through the blood-brain barrier [34]. Additionally, a tissue, particularly an arterial wall, which has the different material properties in each layer, is commonly modeled as a multilayer medium [35, 36].

However, no works have been reported throughout the literature that analytically modeled and evaluated the performance of multilayer DBMC channel from the perspective of communications and an information theory. It is still not
clear how molecules will propagate through the multilayer DBMC channel that is consisting of different medium properties or different medium temperature. Thus, it is utmost important to develop a mathematical model to predict the concentration profile over time and characterize how molecules will propagate over a multilayer channel. Modeling and analysis of molecules’ propagation over a multilayer channel with different medium properties are important to be explored in order to support the future biomedical applications such as regulating the release of drugs over a multilayer structure of environment in living tissue, as well as for the BANs and IoBNT applications. Therefore, this research work is proposed to model and evaluate the performance of multilayer DBMC channel.

1.3 Research Objectives

The main objective of this research is to mathematically model and evaluate the performance of multilayer DBMC channel. This research study has the following specific objectives:

(i) To develop a mathematical model of multilayer DBMC channel in deriving a closed-form expression of the mean molecular concentration at the RN location.

(ii) To formulate channel characteristics of multilayer DBMC channel.

(iii) To evaluate the performance of the multilayer DBMC channel generated from different medium properties.

1.4 Research Scopes

In order to achieve the objectives, the following scopes have been employed:

(i) The research focuses on mathematical modeling of a point to point (a pair of nanomachines) DBMC channel without any noise sources or propagation impairments to derive the mean molecular concentration at the RN location over a multilayer channel. Furthermore, the propagation of molecules from the point-source TN to the point and passive RN is governed by the Fick’s law of diffusion.
(ii) Pulse-based modulation (an impulsive transmission) with concentration encoding scheme as well as amplitude detection technique is considered in formulating the multilayer DBMC channel characteristics such as channel impulse response, channel time delay, channel attenuation or the maximum amplitude of mean molecular concentration, channel delay spread, and channel capacity.

(iii) The performance evaluation is done for multilayer diffusion over the air-water-blood plasma medium representing the simplified model of the alveolar-blood capillary barriers in the human respiration system. The interlayer between two different mediums and membranes is considered thin and permeable to the transmitted information molecules which have a radius similar to an oxygen atom.

The detailed explanations on the assumptions made in mathematical modeling of multilayer DBMC channel are given in Chapter 4. Thus, the developed mathematical model has the following limitations:

(i) The mean molecular concentration at the RN location is derived for a point-source TN and a point-source RN with an infinite boundary. For more realistic and accurate models, propagation of molecules between a spherical TN and a spherical RN in a confined medium needs to be considered in the future [37].

(ii) The propagation of molecules in the 3-D environment over a multilayer channel is without any reaction and drift velocity. Therefore, the movement of molecules is subjected to a free diffusion from the higher concentration region to the lower concentration region [7, 38], and the viscous forces within the medium dominate the propagation process [38–40]. In other words, the derived closed-form equation is not considered for the cases when the concentration of molecules is very high compared to the medium molecules, and the collisions between molecules affect their movement.

(iii) The developed mathematical model is independent of any noise exists in the DBMC system such as sampling noise at the TN [13], diffusion or Brownian noise due to randomness propagation of molecules [13, 38], and reception or residual noise at the RN [38, 41].

(iv) Modeling of the ligand-binding reception and decoding process at the RN is beyond the scope of this research. In this work, an amplitude detection scheme is considered, where bits '1' and '0' represented by the higher and the lower concentration of molecules inside the RN sensing volume.
1.5 Research Contributions

The contributions of this research work are as follows:

(i) A derived closed-form equation of mean molecular concentration for multilayer DBMC channel.

In this work, the diffusive flux of molecules in single layer medium is interpreted analogously to Ohm’s law. The electrical current, $I$ in Ohm’s law represents the diffusion flux of molecules, $J(r, t)$, the electrical resistance, $R$ represents the total length per unit diffusion coefficient, $\ell/D$ or diffusive resistance of the medium, and the voltage difference, $(v_0 - v_1)$ represents the concentration difference, $c(r_0, t) - c(r_0 + \ell, t)$ of the information molecules between two points [42]. Then, a multilayer channel of DBMC is modeled as an $n$-resistor in series where the average diffusive flux of molecules over a multilayer medium is obtained by adding the diffusive resistance of each layer analogous to the addition of series resistors in electrical circuit theory as proposed in [43]. By considering a conservation law of molecules, the partial differential equation (PDE) of time rate change at distance, $r$ and time $t$ of molecular concentration over a multilayer medium is obtained from the average diffusive flux and the continuity equations. Finally, the closed-form equation of mean molecular concentration for multilayer DBMC channel is derived by finding the solution of the PDE for an impulsive transmission of molecules using the Fourier and Laplace transforms method.

It is found that the mean molecular concentration of multilayer DBMC is dependent on the total number of transmitted molecules, transmission distance, and an average diffusion coefficient. In addition, the average diffusion coefficient is inversely proportional to the summation of each layer fraction per layer diffusion coefficient.

(ii) A formulated closed-form equation of channel characteristics of multilayer DBMC channel in terms of channel impulse response, channel time delay, channel attenuation, channel delay spread, and channel capacity.

Channel delay spread expression for multilayer DBMC channel is derived by considering 10 dB below the maximum peak of mean molecular concentration as the minimum level using the MAPLE software. The delay spread is obtained by subtracting two-time instants at which the mean molecular concentration equals one-tenth of the maximum peak of mean molecular concentration or channel attenuation. In this work, the maximum
peak of mean molecular concentration is obtained by substituting time delay into the closed-form equation of mean molecular concentration. While, the time delay is obtained by finding the time instant at which the time derivative of the closed-form equation of mean molecular concentration is equal to zero.

In summary, both time delay and delay spread are directly proportional to the square of transmission distance and inversely proportional to the average diffusion coefficient. Moreover, the channel attenuation is directly proportional to the number of transmitted molecules and is inversely proportional to the cube of transmission distance.

In addition, a capacity expression for multilayer DBMC channel is also derived in this research work. The entropy of the number of transmitted molecules per time sample of transmitted signal is obtained by modeling the time function of the transmitted signal as a band-limited ensembles function within a bandwidth, \( W \). By performing Fourier transforms, variable substitution, manipulating the integration part, and simplification using de Moivre’s formula, the transfer function Fourier transform of the channel impulse response is obtained. This equation is then used to determine the conditional entropy per second of the transmitted signal given the received signal as well as the expression of mutual information of multilayer DBMC channel. Finally, the capacity expression is obtained by maximizing the mutual information between the transmitted signal and the received signal with respect to the probability density function of the transmitted signal.

The capacity of multilayer DBMC is dependent on the bandwidth of transmitted signal, an average thermodynamic power spent by the TN to transmit molecules, a temperature of the system, transmission distance, and the average diffusion coefficient. The capacity is linearly dependent on the bandwidth of transmitted signal. However, the upper and lower bound of capacity are affected by the transmission distance and the average diffusion coefficient of multilayer medium.

(iii) Performance analysis of multilayer DBMC channel due to different medium properties.

Performance analysis of multilayer DBMC channel in terms of channel attenuation, channel time delay, and channel delay spread for different layer fraction, transmission distance, and the number of transmitted molecules is evaluated analytically using MATLAB software. In addition, numerical evaluation of the effects of parameter variation such as an average thermodynamic power for molecule transmission, the bandwidth of the
transmitted signal, transmission distance, and layer fraction on the capacity of multilayer DBMC channel are also presented and discussed.

In general, it is found that the impulse responses of multilayer DBMC channel rapidly increases from zero to a maximum peak and then decrease over time, forming a long tail and approaching zero as $t$ becomes infinity. Moreover, the higher average diffusion coefficient, the faster the rate of the mean number of received molecules reaching its maximum peak and the shorter the channel delay spread. The results also show that doubling the transmission distance increases both time delay and delay spread by four-fold, and decreases the maximum peak or channel attenuation by eight-fold. In addition, increasing the number of molecules increases the maximum peak of mean molecular concentration; however, the delay spread and pulses spreading as well as time delay remains unchanged. The numerical results showed that the wider the transmission bandwidth, the higher the channel capacity, and the shorter transmission distance, the higher the channel capacity. Increasing the average transmitted power increases the channel capacity as well.

1.6 Significance of Research

The findings from this research work are valuable as a foundation in the development and fabrication of future artificial nanocommunication and networks system, which involves the propagation of molecules through a multilayer medium. Mathematical models of the molecular communication system will allow a researcher to perform mathematical analysis, design and optimization on molecular communication systems. It is expected that performance evaluations of the study provide insight to help engineers in developing or realizing the multilayer DBMC system due to different medium properties.

1.7 Thesis Outline

The entire structure of the thesis is organized into six chapters. A brief overview of research background and information related to the research work such as problem statement, research objectives, scopes of research, research contributions, and the importance of the work are addressed in Chapter 1.
REFERENCES


63. Unluturk, B. D., Pehlivanoglu, E. B. and Akan, O. B. Molecular Channel Model with Multiple Bit Carrying Molecules. *2013 First International Black*


75. Mahfuz, M. U., Makrakis, D. and Mouftah, H. T. Characterization


