

MODELING AND ANALYSIS OF MOLECULAR COMMUNICATION SYSTEMS

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MODELING AND ANALYSIS OF MOLECULAR COMMUNICATION SYSTEMS

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Certificate

This is to certify that the thesis entitled "**Modeling and Analysis of Molecular Communication Systems**" being submitted by **Mr. Ankit** to the Department of Electrical Engineering, Indian Institute of Technology Delhi, for the award of the degree of **Doctor of Philosophy** is the record of the bona-fide research work carried out by him under my supervision. In my opinion, the thesis has reached the standards fulfilling the requirements of the regulations relating to the degree.

The results contained in this thesis have not been submitted either in part or in full to any other university or institute for the award of any degree or diploma.

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Abstract

Molecular communication (MC) is a communication technique that utilizes Brownian entities as information carriers. Apart from being suitable for various environments where conventional electromagnetic and optical wave transmissions are not efficient means of communication, MC has several applications in the fields of synthetic biology, animal behavior studies, bio-nanotechnology, systems biology, targeted drug delivery, the internet of Bio-Nano things and many other scientific disciplines. Contrary to having such a huge potential, the research in the MC domain is still in its nascent stage. One of the primary reasons for such a lag in the MC research is the lack of theoretical and analytical models and techniques that can characterize a given MC system. These models are needed for evaluating the performance of the MC system under the assumptions of various Brownian entities that are propagating in different fluid enclosures and are received by distinct molecular receivers. In the absence of suitable analytical techniques for MC channel characterization and performance evaluation, researchers have relied heavily on simulations; which are generally time-consuming and do not provide readily available mathematical expressions for intuitive insights. Thus, in this dissertation, we perform analytical modeling and mathematical performance evaluation of various MC systems.

The study begins with the performance evaluation of MC systems that can be modeled by using one-dimensional (1-D) channel characterizations. The performance evaluation of a generalized M -ary modulated molecular signal that is propagating in a diffusive-drift fluid environment is provided. Arrival modeling of the molecules at the absorbing receiver is done by using a Poisson random variable. A lower bound on the capacity of the aforementioned MC system is obtained, and the symbol error rates

are also evaluated. Next, we provide a communication perspective to the cell signaling established using Boolean AND and OR logic gates. The cell signaling between molecular sources and effector protein that is mediated through the receptor proteins is represented by relay based communication between transmitters and Boolean gate receivers. Error performance and some capacity bounds are evaluated for the Boolean communication system. Furthermore, the relationship between the reliability of a communication link and a disease is also discussed.

We then venture into the area of channel characterizations for different two-dimensional (2-D) and three-dimensional (3-D) MC systems; based on various natural and artificial applications. The analytical formulations of molecular reception probabilities of passive and active receivers for a 3-D diffusive-drift fluid environment are obtained, and a comparison between the performance of the two receivers in terms of error rates is presented. It is observed by analysis and simulations that under the given MC constraints, the active receiver performs better than the passive receiver due to the lesser amount of interference encountered by the former.

Apart from employing passive Brownian particles (e.g., molecules), we also analytically explore MC by using active Brownian particles like bacteria and molecular motor as information entities. A 2-D channel characterization of the bacteria signal in the presence of an absorbing line in a fluid environment is provided by deriving the first hitting time (FHT) probability density function (PDF). A novel method of modeling the interference affected diffusion channel as finite-state Markov channel (FSMC) is proposed, and the capacity of the bacterial communication system is evaluated. For the motor signal, we study its propagation in the presence of an absorbing node by employing a 2-D square lattice structure. The FHT PDF and the hitting probabilities of the motor signal to the absorbing node are derived. Motivated by the neuronal cell signaling applications, we propose to encode the information in the release timing of the motor particle and evaluate the error performance. Criteria to determine the effective memory length of the diffusion channel are also suggested. Furthermore, by quantifying the directivity of a motor signal, it is shown that the directed random walk is better suited for large range MC.

From the unconstrained and semi-constrained fluid environments, we then proceed to analyze MC systems established inside enclosed containers. The spatio-temporal distributions of molecules inside 2-D rectangular and 3-D cuboid containers that have all reflecting walls but one absorbing wall are provided, and the FHT PDFs of the molecules to the respective absorbing walls are derived. Furthermore, the numerical capacity evaluation of a temporally modulated MC system within rectangular and cuboid enclosed boundaries is also provided.

सार

आणविक संचार (एमसी) एक संचार तकनीक है जो सूचना वाहक के रूप में ब्राउनियन कणों का उपयोग करती है। विभिन्न वातावरणों के लिए उपयुक्त होने के अलावा, जहां पारंपरिक विद्युत चुम्बकीय और ऑप्टिकल वेव प्रसारण संचार के कुशल साधन नहीं हैं, एमसी के सिंथेटिक जीव विज्ञान, पशु व्यवहार अध्ययन, जैव-नैनो-प्रौद्योगिकी, सिस्टम जीव विज्ञान, लक्षित दवा वितरण, जैव नैनो चीजों का इंटरनेट और कई अन्य वैज्ञानिक विषयों में बहुत से अनुप्रयोग हैं। इतनी बड़ी क्षमता होने के विपरीत, एमसी डोमेन में शोध अभी भी अपने नवजात चरण में है। एमसी अनुसंधान में इस तरह की अपरिपक्वता के प्राथमिक कारणों में से एक सैद्धांतिक और विश्लेषणात्मक मॉडल और तकनीकों की कमी है जो दिए गए एमसी सिस्टम पर निर्भर करती है। इन मॉडलों की आवश्यकता विभिन्न एमसी प्रणालियों के प्रदर्शन का मूल्यांकन करने के लिए आवश्यक है, जिनमें विभिन्न ब्राउनियन कणों का प्रसारण विभिन्न द्रव बाड़ों में हो रहा है और यह ब्राउनियन कण विभिन्न आणविक रिसीवरों द्वारा प्राप्त किए जा रहे हैं। एमसी चैनल लक्षण वर्णन और प्रदर्शन मूल्यांकन के लिए उपयुक्त विश्लेषणात्मक तकनीकों की अनुपस्थिति में, शोधकर्ताओं ने सिमुलेशन पर निर्भरता दिखाई है; जो आमतौर पर समय लेने वाली होती है और सहज ज्ञान युक्त अंतर्दृष्टि के लिए आसानी से उपलब्ध गणितीय अभिव्यक्ति प्रदान नहीं करती हैं। इस प्रकार, इस शोध प्रबंध में, हम विभिन्न एमसी सिस्टम के विश्लेषणात्मक मॉडलिंग और गणितीय प्रदर्शन मूल्यांकन करते हैं।

यह अध्ययन एमसी सिस्टम के प्रदर्शन मूल्यांकन के साथ शुरू होता है जिसे एक-आयामी (1-डी) चैनल लक्षण वर्णन का उपयोग करके मॉडल किया जा सकता है। एक सामान्यीकृत *M-ary* संग्राहक आणविक संकेत का प्रदर्शन मूल्यांकन प्रदान किया जाता है जो एक विसारक-बहाव द्रव वातावरण में प्रचारित हो रहा है। अब्सॉर्बिंग रिसीवर पर अणुओं का आगमन मॉडलिंग एक पॉइसन यादृच्छिक चर का उपयोग करके किया जाता है। उपरोक्त एमसी प्रणाली की संचार-क्षमता पर एक निचली बाध्यता प्राप्त की जाती है, और प्रतीक त्रुटि दर का भी मूल्यांकन किया जाता है। इसके बाद, हम बूलियन तथा और लॉजिक गेट्स का उपयोग करके स्थापित सेल सिग्नलिंग को एक संचार परिप्रेक्ष्य प्रदान करते हैं। रिसेप्टर प्रोटीन के माध्यम से मध्यस्थता करने वाले आणविक स्रोतों और प्रभावकारी प्रोटीन के बीच सेल सिग्नलिंग को ट्रांसमीटर और बूलियन गेट रिसीवर के बीच रिले आधारित संचार द्वारा दर्शाया जाता है। बूलियन संचार प्रणाली के लिए त्रुटि प्रदर्शन और कुछ संचार-क्षमता सीमा का मूल्यांकन किया जाता है। इसके अलावा, संचार लिंक की विश्वसनीयता और एक बीमारी के बीच संबंध पर भी चर्चा की गई है।

फिर हम विभिन्न दो-आयामी (2-डी) और तीन-आयामी (3-डी) एमसी सिस्टम के लिए चैनल लक्षण वर्णन के क्षेत्र में उद्यम करते हैं जो कि विभिन्न प्राकृतिक और कृत्रिम अनुप्रयोगों पर आधारित है। 3-डी विसारक-बहाव द्रव पर्यावरण के लिए निष्क्रिय और सक्रिय रिसीवर की आणविक रिसेप्शन संभावनाओं के विश्लेषणात्मक सूत्र प्राप्त किए जाते हैं, और त्रुटि दर के संदर्भ में दो रिसीवरों के प्रदर्शन के बीच तुलना प्रस्तुत की जाती है। यह विश्लेषण और सिमुलेशन द्वारा देखा गया है कि दिए गए एमसी

बाधाओं के तहत, सक्रिय रिसीवर निष्क्रिय रिसीवर की तुलना में बेहतर प्रदर्शन करता है क्योंकि सक्रिय रिसीवर में कम हस्तक्षेप होता है।

निष्क्रिय ब्राउनियन कणों (जैसे, अणु) को नियोजित करने के अलावा, हम सक्रिय रूप से बैक्टीरिया और आणविक मोटर जैसे सक्रिय ब्राउनियन कणों का उपयोग करके सूचना संस्थाओं के रूप में एमसी का पता लगाते हैं। एक तरल वातावरण में एक अवशोषित लाइन की उपस्थिति में बैक्टीरिया सिग्नल का 2-डी चैनल लक्षण वर्णन पहले हिटिंग समय (एफएचटी) की संभावना वितरण फ़ंक्शन (पीडीएफ) को प्राप्त करके प्रदान किया जाता है। परिमित राज्य मार्कोव चैनल (एफएसएमसी) के रूप में हस्तक्षेप प्रभावित प्रसार चैनल मॉडलिंग की एक नई विधि प्रस्तावित की गयी है, और जीवाणु संचार प्रणाली की संचार-क्षमता का मूल्यांकन किया गया है। मोटर सिग्नल के लिए, हम 2-डी वर्ग जाली संरचना को नियोजित करके एक अवशोषित नोड की उपस्थिति में इसके प्रसार का अध्ययन करते हैं। एफएचटी पीडीएफ और अवशोषित नोड के लिए मोटर सिग्नल की मार संभावनाएं व्युत्पन्न हैं। न्यूरोनल सेल सिग्नलिंग अनुप्रयोगों द्वारा प्रेरित, हम मोटर कण की रिहाई के समय में जानकारी को एन्कोड करने और त्रुटि प्रदर्शन का मूल्यांकन करने का प्रस्ताव करते हैं। प्रसार चैनल की प्रभावी स्मृति लंबाई निर्धारित करने के लिए मानदंड भी सुझाए गए हैं। इसके अलावा, एक मोटर सिग्नल की प्रत्यक्षता की मात्रा निर्धारित करके, यह दिखाया गया है कि निर्देशित यादृच्छिक चलना बड़ी रेंज एमसी के लिए बेहतर है।

असीम और अर्ध-असीम द्रव वातावरण से, हम फिर संलग्न पात्रों के अंदर स्थापित एमसी सिस्टम का विश्लेषण करने के लिए आगे बढ़ते हैं। 2-डी आयताकार और 3-डी घनाभ पात्रों के अंदर अणुओं के अनुपात-अस्थायी वितरण, जिनमें सभी प्रतिबिंबित दीवारें हैं, लेकिन एक अवशोषित दीवार है, प्रदान की जाती है, और अणुओं के एफएचटी पीडीएफ प्राप्त किए जाते हैं। इसके अलावा, आयताकार और घनाभ से परिबद्ध सीमाओं के भीतर एक अस्थायी रूप से संशोधित एमसी प्रणाली का संख्यात्मक संचार-क्षमता मूल्यांकन भी प्रदान किया जाता है।

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Abbreviations

1-D	One-Dimensional
2-D	Two-Dimensional
3-D	Three-Dimensional
AF	Amplify-and-Forward
ASEP	Average Symbol Error Probability
ATP	Adenosine Triphosphate
CDF	Cumulative Distribution Function
CRT	Controlled Release Technology
CSIR	Channel Side Information at the Receiver
CSK	Concentration Shift Keying
DA	Deterministic Annealing
DF	Decode-and-Forward
DNA	Deoxyribonucleic Acid
EF	Estimate-and-Forward
FHT	First Hitting Time
F-P	Fokker-Planck
FSMC	Finite-State Markov Channel
HMM	Hidden Markov Model
ILI	Inter-Link Interference
ISI	Inter-Symbol Interference
LHS	Left-Hand Side
LOC	Lab-on-a-Chip
LOS	Line-of-Sight

MAP	Maximum a Posteriori
MC	Molecular Communication
MCA	Maxentropic Capacity-Approaching
MIMO	Multiple-Input Multiple-Output
miRNA	Micro Ribonucleic Acid
MISO	Multiple-Input Single-Output
ML	Maximum Likelihood
MLD	Maximum Likelihood Detector
mRNA	Messenger Ribonucleic Acid
MSE	Mean-Square Error
PDF	Probability Density Function
PMF	Probability Mass Function
RHS	Right-Hand Side
RNA	Ribonucleic Acid
RPD	Rapid Pathogen Diagnostics
SDE	Stochastic Differential Equation
SEP	Symbol Error Probability
SIMO	Single-Input Multiple-Output
SISO	Single-Input Single-Output
VSDA	Viterbi Sequence Detection Algorithm
w.r.t.	with respect to