

**CAPACITY ANALYSIS AND INTERFERENCE
MITIGATION TECHNIQUES FOR
DIFFUSION-BASED MOLECULAR
COMMUNICATION SYSTEMS**

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Capacity Analysis and Interference Mitigation Techniques for Diffusion-Based Molecular Communication Systems

by

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Certificate

This is to certify that the work presented in this thesis entitled "**Capacity Analysis and Interference Mitigation Techniques for Diffusion-Based Molecular Communication Systems**" being submitted by **Ms. Muskan Ahuja** to Bharti School Of Telecommunication Technology and Management, **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 her 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

Nanotechnology is a revolutionary paradigm for the future of medical applications. The theory of miniaturization has played a pivotal role in the emergence of nanotechnology and biotechnology. The development of micro and nano scale devices is facilitated by the tools provided by nanotechnology. Nanomachines are the basic functional devices with nanoscale size and little complexity. Therefore, they can accomplish only simple tasks like communicating, computing, sensing, data storage, and actuation. Due to their limited functionality and scarce energy resource, nanomachines need to work cooperatively to achieve a wide range of applications including healthcare, industrial, environmental, etc. Nano-communication enables communication between a group of nanomachines to achieve a specific task. Such nanoscale communication can be implemented using electromagnetic (EM), nanomechanical, acoustic, and molecular communication (MC) techniques. Owing to the non-invasiveness and biocompatibility, MC stands out as the most suitable communication paradigm for nanomachine networks, i.e., nanonetworks.

MC is a gifted technique inspired by nature-based communication where information is passed using molecules from sender to receiver. For instance, the human body is a complex network of communicating nanomachines performing a specific function. Motivated by nature, artificial nanonetworks can be formed using synthetic biology for spurring a wider range of biomedical and industrial applications. MC has gained enormous attention from researchers in the past decade still, the research is in its infancy. The key challenges include, inter alia, efficient information transmission through encoding and decoding strategies, lack of end-to-end realistic MC model, propagation of information molecules in a controlled manner, and the highly stochastic nature of

MC channel. Therefore, in this dissertation, we evaluate realistic end-to-end MC system using capacity and bit error rate (BER) analysis alongwith providing performance analysis of MC system models utilizing different modulation schemes.

We first present the end-to-end biochemical MC model with the finite number of receptors on the receiver's boundary. The capacity and performance analysis for the aforementioned system model is carried out using the Markov chain. The probability of binding and unbinding of molecules on the receiver's surface depends on the concentration of molecules in the vicinity of the receiver (Rx). Therefore, the Rx is modeled using a two-state Markov chain, where one state is bind and the other state is unbind.

We next move to the study of multiple-input multiple-output (MIMO) modulation techniques in MC system. In order to achieve a high data rate, MIMO systems prove to be beneficial for MC systems. Unlike single-input single-output (SISO) systems, MIMO systems suffer greatly from inter-link interference (ILI) alongwith inter-symbol interference (ISI). The spatial modulation (SM) schemes have shown enormous benefits in terms of their simplicity, high spectral efficiency, and low energy consumption in MIMO-MC systems. One benchmark SM scheme in MC literature is molecular space shift keying (MSSK) where information is transmitted using antenna indices of the transmitter (Tx) nanomachine. We extend this study to propose a coded index modulation (IM) strategy named molecular spatio-temporal coded modulation (MSTCM) where information is judiciously transferred using antenna index selection. The antenna index in the present interval is judiciously activated in accordance with the antenna activated in the previous symbol interval. The proposed scheme is shown to mitigate ISI and ILI problems better than the benchmark MSSK modulation scheme. Moreover, the analytical BER expression is derived which very well corroborates with the simulated one.

We then embed the pulse position modulation (PPM) strategy in the MSTCM modulation scheme to form a position molecular spatio-temporal coded modulation (PMSTCM) scheme. It is proved by simulations and analytical results that PMSTCM better alleviates the problem of ISI and ILI in molecular MIMO systems. Until now, the proposed molecular schemes transmit information using a single antenna index in

one symbol interval. For enhancing the system throughput, a fixed number of antennas on the Tx side can be activated for transferring information. This calls for generalized space shift keying modulation schemes for molecular MIMO systems. Motivated by conventional radio-based communication, we illustrated the generalized molecular space shift keying (GMSSK) scheme for two activated antennas on the Tx side and compared it with the benchmark MSSK and other modulation strategies considering the same symbol interval. The study depicts that GMSSK outperforms existing molecular MIMO modulation schemes for a majority of bit durations.

अमूर्त

चिकित्सा अनुप्रयोगों के भविष्य के लिए नैनोटेक्नोलॉजी एक क्रांतिकारी प्रतिमान है। लघुकरण के सिद्धांत ने नैनो प्रौद्योगिकी और जैव प्रौद्योगिकी के उद्भव में महत्वपूर्ण भूमिका निभाई है। सूक्ष्म और नैनो पैमाने के उपकरणों का विकास नैनोटेक्नोलॉजी द्वारा उपलब्ध कराए गए उपकरणों द्वारा सुगम होता है। नैनोमशीनें नैनोस्केल आकार और थोड़ी जटिलता वाले बुनियादी कार्यात्मक उपकरण हैं। इसलिए, वे केवल संचार, कंप्यूटिंग, सेंसिंग, डेटा स्टोरेज और एक्जुएशन जैसे सरल कार्य ही पूरा कर सकते हैं। उनकी सीमित कार्यक्षमता और दुर्लभ ऊर्जा संसाधन के कारण, नैनोमशीनों को स्वास्थ्य देखभाल, औद्योगिक, पर्यावरण आदि सहित अनुप्रयोगों की एक विस्तृत श्रृंखला को प्राप्त करने के लिए सहयोगात्मक रूप से काम करने की आवश्यकता होती है। नैनो-संचार एक विशिष्ट कार्य को प्राप्त करने के लिए नैनोमशीनों के समूह के बीच संचार को सक्षम बनाता है। इस तरह के नैनोस्केल संचार को विद्युत चुम्बकीय (ईएम), नैनोमैकेनिकल, ध्वनिक और आणविक संचार (एमसी) तकनीकों का उपयोग करके कार्यान्वित किया जा सकता है। गैर-आक्रामकता और जैव-अनुकूलता के कारण, एमसी नैनोमशीन नेटवर्क, यानी नैनो नेटवर्क के लिए सबसे उपयुक्त संचार प्रतिमान के रूप में सामने आता है।

एमसी प्रकृति-आधारित संचार से प्रेरित एक प्रतिभाशाली तकनीक है जहां प्रेषक से प्राप्तकर्ता तक अणुओं का उपयोग करके सूचना प्रसारित की जाती है। उदाहरण के लिए, मानव शरीर एक विशिष्ट कार्य करने वाली नैनोमशीनों का संचार करने का एक जटिल नेटवर्क है। प्रकृति से प्रेरित होकर, बायोमेडिकल और औद्योगिक अनुप्रयोगों की एक विस्तृत श्रृंखला को बढ़ावा देने के लिए सिंथेटिक जीवविज्ञान का उपयोग करके कृत्रिम नैनोनेटवर्क का निर्माण किया जा सकता है। एमसी ने पिछले दशक में शोधकर्ताओं का काफी ध्यान आकर्षित किया है, अभी भी शोध अपनी प्रारंभिक अवस्था में है। प्रमुख चुनौतियों में, अन्य बातों के साथ-साथ, एन्कोडिंग और डिकोडिंग रणनीतियों के माध्यम से कुशल सूचना प्रसारण, एंड-टू-एंड यथार्थवादी एमसी मॉडल की कमी, नियंत्रित तरीके से सूचना अणुओं का प्रसार और एमसी चैनल की अत्यधिक स्टोकेस्टिक प्रकृति शामिल हैं। इसलिए, इस शोध प्रबंध में, हम विभिन्न मॉड्यूलेशन योजनाओं का उपयोग करते हुए एमसी सिस्टम मॉडल के प्रदर्शन विश्लेषण प्रदान करने के साथ-साथ क्षमता और बिट त्रुटि दर (बीईआर) विश्लेषण का उपयोग करके यथार्थवादी एंड-टू-एंड एमसी सिस्टम का मूल्यांकन करते हैं।

हम पहले रिसीवर की सीमा पर रिसेप्टर्स की सीमित संख्या के साथ एंड-टू-एंड बायोकेमिकल एमसी मॉडल प्रस्तुत करते हैं। उपरोक्त सिस्टम मॉडल के लिए क्षमता और प्रदर्शन विश्लेषण मार्कोव श्रृंखला का उपयोग करके किया जाता है। रिसीवर की सतह पर अणुओं के जुड़ने और खुलने की संभावना रिसीवर के आसपास अणुओं की सांद्रता (आरएक्स) पर निर्भर करती है। इसलिए, आरएक्स को दो-राज्य मार्कोव श्रृंखला का उपयोग करके तैयार किया गया है, जहां एक राज्य बाइंड है और दूसरा राज्य अनबाइंड है।

अब हम एमसी सिस्टम में मल्टीपल-इनपुट मल्टीपल-आउटपुट (एमआईएमओ) मॉड्यूलेशन तकनीकों के अध्ययन की ओर बढ़ते हैं। उच्च डेटा दर प्राप्त करने के लिए, MIMO सिस्टम MC सिस्टम के लिए फायदेमंद साबित होते हैं। सिंगल-इनपुट सिंगल-आउटपुट (SISO) सिस्टम के विपरीत, MIMO सिस्टम इंटर-लिंक इंटरफेरेंस (ILI) के साथ-साथ इंटर-सिंबल इंटरफेरेंस (ISI) से बहुत प्रभावित होते हैं। स्थानिक मॉड्यूलेशन (एसएम) योजनाओं ने एमआईएमओ-एमसी प्रणालियों में उनकी सादगी, उच्च वर्णक्रमीय दक्षता और कम ऊर्जा खपत के मामले में भारी लाभ दिखाया है। एमसी साहित्य में एक बेंचमार्क एसएम योजना आणविक अंतरिक्ष शिफ्ट कुंजीयन (एमएसएसके) है जहां ट्रांसमीटर (टीएक्स) नैनोमशीन के एंटीना सूचकांकों का उपयोग करके सूचना प्रसारित की जाती है। हम आणविक अनुपात-अस्थायी कोडित मॉड्यूलेशन (एमएसटीसीएम) नामक एक कोडित सूचकांक मॉड्यूलेशन (आईएम) रणनीति का प्रस्ताव करने के लिए इस अध्ययन का विस्तार करते हैं जहां एंटीना इंडेक्स चयन का उपयोग करके जानकारी को विवेकपूर्ण ढंग से स्थानांतरित किया जाता है। वर्तमान अंतराल में एंटीना सूचकांक पिछले प्रतीक अंतराल में सक्रिय एंटीना के अनुसार विवेकपूर्ण ढंग से सक्रिय होता है। प्रस्तावित योजना को बेंचमार्क एमएसएसके मॉड्यूलेशन योजना की तुलना में आईएसआई और आईएलआई समस्याओं को बेहतर ढंग से कम करने के लिए

दिखाया गया है। इसके अलावा, विश्लेषणात्मक बीईआर अभिव्यक्ति प्राप्त की गई है जो सिम्युलेटेड के साथ बहुत अच्छी तरह से पुष्टि करती है।

फिर हम स्थिति आणविक अनुपात-अस्थायी कोडित मॉड्यूलेशन (पीएमएसटीसीएम) योजना बनाने के लिए एमएसटीसीएम मॉड्यूलेशन योजना में पल्स स्थिति मॉड्यूलेशन (पीपीएम) रणनीति को एम्बेड करते हैं। सिमुलेशन और विश्लेषणात्मक परिणामों से यह साबित हुआ है कि पीएमएसटीसीएम आणविक एमआईएमओ प्रणालियों में आईएसआई और आईएलआई की समस्या को बेहतर ढंग से कम करता है। अब तक, प्रस्तावित आणविक योजनाएं एक प्रतीक अंतराल में एकल एंटीना सूचकांक का उपयोग करके सूचना प्रसारित करती हैं। सिस्टम थ्रूपुट को बढ़ाने के लिए, सूचना स्थानांतरित करने के लिए टीएक्स साइड पर एक निश्चित संख्या में एंटेना को सक्रिय किया जा सकता है। इसके लिए आणविक एमआईएमओ प्रणालियों के लिए सामान्यीकृत स्पेस शिफ्ट कुंजीयन मॉड्यूलेशन योजनाओं की आवश्यकता होती है। पारंपरिक रेडियो-आधारित संचार से प्रेरित होकर, हमने टीएक्स पक्ष पर दो सक्रिय एंटेना के लिए सामान्यीकृत आणविक अंतरिक्ष शिफ्ट कुंजीयन (जीएमएसएसके) योजना का चित्रण किया और समान प्रतीक अंतराल पर विचार करते हुए बेंचमार्क एमएसएसके और अन्य मॉड्यूलेशन रणनीतियों के साथ इसकी तुलना की। अध्ययन से पता चलता है कि जीएमएसएसके अधिकांश बिट अवधि के लिए मौजूदा आणविक एमआईएमओ मॉड्यूलेशन योजनाओं से बेहतर प्रदर्शन करता है।

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Abbreviations

ATD	Adaptive Threshold Detector
BCSK	Binary Concentration Shift Keying
BER	Bit Error Rate
BIND	Binding in Discrete Time
CIR	Channel Impulse Response
CSI	Channel State Information
DBMC	Diffusion-Based Molecular Communication
DB-MoMIMO	Diffusion-Based Molecular Multiple-Input Multiple-Output
DbOMC	Diffusion-Based ON-OFF Keying Molecular Communication
EM	Electromagnetic
FTD	Fixed Threshold Detector
GMSSK	Generalized Molecular Space Shift Keying
IID	Independent and Identically Distributed
ILI	Inter-Link Interference
IM	Index Modulation
IoBNT	Internet of Bio-Nano Things
IoT	Internet of Things
ISI	Inter-Symbol Interference
LSB	Least Significant Bit
MC	Molecular Communication
MI	Mutual Information
MCD	Maximum Count Decoder
MIMO	Multiple-Input Multiple-Output

MISO	Multiple-Input Single-Output
MSB	Most Significant Bit
MSM	Molecular Spatial Modulation
MSSK	Molecular Space Shift Keying
MSTCM	Molecular Spatio-Temporal Coded Modulation
MTSK	Molecular Transition Shift Keying
OOK	On-Off Keying
PDF	Probability Density Function
PMSTCM	Position Molecular Spatio-Temporal Coded Modulation
PPM	Pulse Position Modulation
QMSSK	Quadrature Molecular Space Shift Keying
RDME	Reaction-Diffusion Master Equation with Exogenous Input
R.H.S	Right Hand Side
Rx	Receiver
SISO	Single-Input Single Output
SM	Spatial Modulation
SMUX	Spatial Multiplexing
SOP	Sum Of Product
SSK	Space Shift Keying
Tx	Transmitter
UCA	Uniform Circular Array

Notations

Parameter	Definition
α_S	Transition probability from inactive to active state of the ligand receptor
A	Active state of the receptor
$\mathcal{A}$	Set of available Tx antenna indices
β	Probability of transition from active to inactive receptor state
$\mathcal{B}$	Set of allowable antenna indices
C	Capacity
C_{IID}	IID capacity of ligand channel
d	Distance between transmitter and receiver
$d_H(a, b)$	Hamming distance between the bit sequences a and b
d_q	Distance between antennas of a particular antenna pair
d_r	Distance between centre of the Rx circular array and Rx's surface projection
D	Diffusion coefficient
D_l	Total decoding length of the symbol sequence
$f_{\mathbb{L}}(\alpha_S)$	Probability for $\mathbb{L}$ to $\mathbb{L}$ State transition of output Y given input S
$f_{\mathbb{L}}^C(\alpha_S)$	1- $f_{\mathbb{L}}(\alpha_S)$
$f_{\mathbb{H}}(\alpha_S)$	Probability for $\mathbb{H}$ to $\mathbb{H}$ State transition of output Y given input S
$f_{\mathbb{H}}^C(\alpha_S)$	1- $f_{\mathbb{H}}(\alpha_S)$
$F_{k,l}^{HIT}(t)$	The probability that the molecules from k^{th} to l^{th} antenna reach before t^{th} time
$h_{k,l}[n]$	n^{th} channel gain for k^{th} Tx antenna and l^{th} Rx antenna
H	Entropy function
$\mathcal{H}(p)$	$-p \log p - (1 - p) \log(1 - p)$
$\mathcal{H}(S)$	Entropy rate of Markov process S

I	Inactive state of the receptor
$\mathcal{I}(S; Y)$	Mutual information rate between S and Y
L	ISI length
μ_P	Mean of normally distributed random variable
μ_C	Mean of normally distributed random variable N_C
$\mu_l[t]$	Mean number of molecules received at l^{th} Rx antenna in t^{th} time interval
N_C	Number of molecules reaching at the input of the receiver in the current interval
N_{HIT}	Number of molecules hitting the receiver surface
N_P	Number of molecules reaching at the input of the receiver in the previous interval
N_R	Number of receptors
N_T	Number of molecules transmitted from the source
$N_{Rx} = N$	Number of antennas at Rx side
$N_{Tx} = N$	Number of antennas at Tx side
Ω	$-p \log p$
$p_S(s)$	Probability of random variable S taking value s
$P_{HIT}(t)$	Probability of getting a molecule by time t
$\mathbf{P}_S$	Probability transition matrix of Markov process S
π_{xy}	Stationary probability of joint process xy
P_e^{IID}	IID BER
P_e^M	Markov BER
P_e	BER
$P_{e J}$	Probability of error given a particular sequence of antennas denoted by J
r	ILI-level
r_r	Radius of spherical receiver antenna
$R_l[t]$	Received number of molecules at l^{th} Rx antenna in t^{th} time interval
$\hat{s}[t]$	Decoded symbol for t^{th} symbol duration
S	Input of the ligand channel
$\mathcal{S}$	Set of all possible allowable antenna sequences
σ_P	Variance of normally distributed random variable N_P
σ_C	Variance of normally distributed random variable N_C

$\sigma_l^2[t]$	Variance of molecules received at l^{th} Rx antenna in t^{th} time interval
t_b	Bit duration
t_s	Symbol duration
τ	Threshold at the input of the receptor to decide between $\mathbb{H}$ or $\mathbb{L}$ input state
τ'	Threshold for number of active sites to decide between $\mathbb{H}$ or $\mathbb{L}$ output state
Δt	Time interval for updating the molecule position
W	Joint Markov process of S and Y
Y	Output of the ligand channel