

# MODELING AND ANALYSIS OF MOLECULAR COMMUNICATION SYSTEMS

## 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.