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RESEARCH ARTICLE

Assessing Molecular Throughput and Efficiency through Simulation in Diffusion-Based Molecular Communication

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Abstract

Objectives: This study investigates the correlation of critical factors influencing throughput and efficiency in diffusion-based molecular communication systems. **Method**: The study presents a simulation model for 3-D diffusion-based molecular communication, incorporating essential parameters such as molecule size, transmission rate, diffusion rate, and transmitter-receiver distance. **Findings**: Through comprehensive simulations, the study reveals the effects of different parameters on throughput and efficiency in diffusion-based molecular communication. It highlights the critical trade-offs associated with system design and optimization. The study reveals the key factors influencing the transmission capabilities, the receiver congestion, and the overall efficiency of the communication system. **Novelty**: In this study, we give a study overview of the latest work of performance metrics in the field of molecular communication. A novel algorithm is proposed to find the throughput and efficiency of molecular communication. The proposed framework analyzes the intricate relationship between system parameters and performance metrics, emphasizing the potential for system optimization. Our simulation work demonstrates how the model parameters influence the performance of the molecular communication system, providing insights for enhancing the system's performance in applications such as targeted drug delivery in the future.

Keywords: Molecular Communication; Diffusion; Transmission Rate; Throughput; Efficiency

1 Introduction

The field of Molecular Communication has gained significant attention as a promising solution for nanoscale communication, enabling communication between biological entities. Molecular communication holds immense potential in a wide array of applications, ranging from biomedical and environmental monitoring to the development of nanoscale sensor networks and targeted drug delivery systems[(1)]. Molecular communication provides precise functioning and enables the implementation of non-invasive and target-specific therapeutic interventions[(2)].

Targeted drug delivery systems are currently a focal point in medical treatments, as they aim to deliver drugs precisely and in a controlled manner to disease sites. Achieving the development of efficient and reliable targeted drug delivery systems based on molecular communication requires a comprehensive understanding of their performance characteristics. Two critical metrics to consider are throughput, which measures the system's capacity to transmit information within a specific time frame, and efficiency, calculated as throughput divided by the transmission rate. In time-sensitive applications like medical diagnostics, high throughput is crucial for ensuring timely and dependable delivery. Efficiency is equally vital, especially when dealing with limited or costly resources such as molecules. However, assessing these performance metrics in molecular communication systems poses a challenge due to the complex interplay of factors like channel characteristics, molecular diffusion properties, and transmission rate.

Our research aims to find the most optimized position achieving both higher dynamic efficiency and throughput. The simulation serves as a comprehensive platform for evaluating molecular communication. It focuses on investigating the impact of factors such as molecule radius, the number of molecules, diffusion rate, and the distance between the transmitter and receiver. The study delves into the associated throughput, measuring molecules received per second, and efficiency, which signifies the ratio of received to transmitted molecules. Our research is dedicated to identifying the optimal configuration and striking a balance that maximizes dynamic efficiency and throughput simultaneously. This exploration contributes valuable insights into the intricate dynamics of molecular communication systems, crucial for advancements in nanoscale communication and applications like targeted drug delivery.

Numerous studies have been documented in the existing literature concerning mathematical models and analysis of performance parameters for MC systems. Lin et al.[3] proposed a high-performance molecular communication system by reducing ISI by estimating distance on maximum likelihood estimation. Nakano et al.[4] focused on the throughput and efficiency of molecular communication nanomachines. The paper derives an upper bound on the throughput and efficiency at a steady state. In further studies, Nakona et al.[5] address the issue of transmission rate control. It discusses the potential problems associated with a high transmission rate, and degradation in efficiency, and presents an optimization problem to address these issues. The paper calculates and presents the optimal transmission rates that maximize throughput and efficiency, showing a trade-off relationship between the two. Felicetti et al.[6] present a communication protocol that enables bidirectional communication, employing techniques like TCP but using implicit acknowledgments to maintain throughput. It includes a connection setup signal, molecule transmission, and a tear-down signal. The protocol's effectiveness is demonstrated through extensive simulations, aiding in the optimization of key parameters.

Wang et al.[7] utilized a decode-and-forward relay technique to expand the communication range and ensure dependable remote communication. Dambari et al.[8] focus on improvement in the performance of MIMO molecular communication systems by lowering path loss. Simulation results are analyzed by the probability of errors and the quantity of molecules representing the signal intensity. Aghababaiyan et al.[9] explore the impact of inter-symbol and co-channel interference on the data rate of molecular communication (MC) systems, focusing on designing an efficient MC system. The research proposes an On/Off keying modulation. By considering inter-symbol interference, the study derives the MC system's data rate. Additionally, the research addresses co-channel interference by suggesting a minimum distance between adjacent MC systems to minimize mutual interference. Awan et al.[10] address the enhancement of communication link performance through the maximization of mutual information between input and output signals. Focusing on molecular communication links employing molecular circuits at both the transmitter and receiver, the study confronts the complexity of this optimization task. The paper derives an expression for mutual information and employs it for numerical maximization. Chouhan et al.[11] explore 3-D molecular communication with moving transmitter and receiver. It derives formulas for hitting rate, detection, false alarm, error probability, and mutual information rate. An optimal threshold is proposed for minimizing error and maximizing information rate. Simulations show that nanomachine mobility can impact error and information rate, but adjusting parameters like threshold and time-slot duration can mitigate this effect. Dhok et al.[12] proposed a cooperative molecular communication system and derived an expression for the maximum achievable rate and probability of error by the AND/OR rule. They also evaluated system performance for uniformly and randomly placed cooperative systems, which are found to be more efficient than the randomly placed systems.

Sajjad et al.[13] described that molecular communication in a vacuum environment can lead to a rise in information transmission rates of about 100 Mbit/s per molecule as feasible. Hoffman et al.[14] emphasize the crucial role of establishing the optimal threshold value for bit decoding in molecular communication systems to minimize bit error rates (BER) and enhance throughput. This research introduces a low-complexity algorithm for determining the optimal threshold in testbeds through a self-adaptive method resulting in significantly reduced BER levels. Moreover, the study demonstrates that existing MC systems can attain an optimal BER, leading to potential error reductions of up to 90%. Bartunik et al.[15] introduce a Neural Network for signal demodulation using concentration shift keying. An 8-symbol modulation alphabet achieves a data rate exceeding 5.5 bits

per second. The constructed neural network can be trained in less than two minutes and is adaptable to varying transmission parameters. Valerio et al.[16] suggested an approach, a symbol detection pipeline, that enhances throughput while maintaining a consistent error rate. The concept is rooted in a machine-learning algorithm. Symbols can be detected reliably, even when confronted with unfamiliar signal-to-noise ratio values. Brand et al.[17] introduce a novel performance measure named area rate efficiency (ARE) that effectively captures the balance between the density of transmission links and inter-user interference (IUI) within multi-link molecular communication systems. Additionally, the paper outlines the process of deriving analytical formulas for channel impulse responses, maximum likelihood detectors, and the determination of the detection threshold. Wang et al.[18] extend previous research which boosts throughput by implementing parallel transmission and sequencing. It utilizes interleaved coding to address bit error rates caused by back-stepping motion, with simulations demonstrating its effectiveness in reducing BER while maintaining DNA information density. The research highlights the potential of high-throughput, low-error DNA-based molecular communication. Brutanik et al.[19] propose neural network-based demodulation techniques that utilize simulated data derived from theoretical channel models and those that rely on real measurements obtained from prototype test beds. Maro et al.[20] focus on the enhancement of molecular communication system efficiency in diverse environments by improving the detection mechanism. The study employed a matched filter to reduce interference, aiming to enhance the detection algorithm for improved Bit Error Rate. Research is also advancing in one of the promising applications of molecular communication in medicine, i.e., targeted drug delivery. Zhao et al.[21] propose an M/M/C/C queue technique for optimum release rate in targeted drug delivery. Through the novel analytical framework, Murugesan et al.[22] focus on the temporal behavior of molecules in the blood, enabling a deeper comprehension of the factors influencing latency. Zhao et al.[23] propose a method that aims to dynamically adjust the rate of drug focus release in response to the varying environmental conditions within the body. Felicetti et al.[24] propose a boundless molecular communication-based propagation model for a blood viscosity monitoring system based on molecular communications. Ponalagusamy et al.[25] describe a mathematical model that elucidates the dynamics of blood flow in arteries exhibiting stenosis. Specifically, the model accounts for variations in peripheral layer thickness along the axial direction and incorporates the influence of variable slip at the arterial wall. Felicetti et al.[26] designed a nanomachine receiver having directionality properties. Kilinc et al.[27] proposed techniques for a receiver within the multicarrier (MC) system to recover transmitted information affected by intersymbol interference (ISI) and noise. Meng et al.[28] designed a molecular communication system taking into account stochastic signaling, arbitrary orders of channel memory, and reception affected by noise.

Supplementary table I gives the comparative study of different performance metrics in the literature. Though a lot of research has been done on performance improvement in molecular communication, very little work has been done on performance metrics such as throughput and efficiency. Considering the significance of this metric in molecular communication applications such as targeted drug delivery, where accurate and precise control of drug delivery is required. This research work focuses on the dependence of different parameters such as transmission rate, molecule radius, diffusion rate, and transmitter-receiver separation on throughput, and efficiency.

2 Methodology

In this study, we consider a three-dimensional fluid environment. As shown in Figure 1, the transmitter is a point source placed at coordinates (0,0,0).

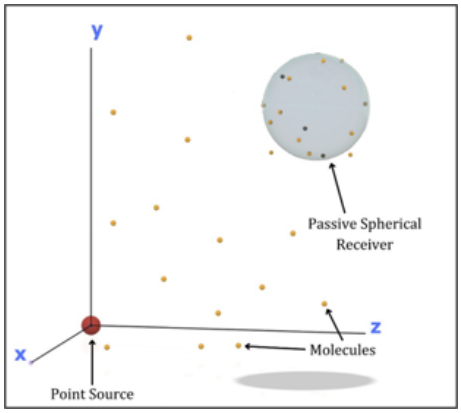

Fig 1. Proposed Molecular Communication System

The transmitter emits N molecules at time t=0 in the environment. A receiver with a radius R_{rx} is placed at position (x, y, z) from the transmitter in 3D space. When a molecule encounters the surface of a receiver, it undergoes absorption and is subsequently eliminated from the surrounding environment. Furthermore, we assume that the molecules diffuse with constant diffusion coefficients D.

The simulation employed Thonny, a Python IDE version 4.1.1, known for its simplicity and efficiency in coding. Various essential libraries enhanced the simulation process, including NumPy for numerical computations, Matplotlib for data visualization, and SciPy for scientific and technical computing. Thonny's user-friendly interface facilitated seamless integration with these libraries, ensuring a robust and versatile simulation environment. The simulations were executed on an HP laptop with an AMD Ryzen 5 3450U processor featuring Radeon Vega Mobile Graphics, operating at a speed of 2.10 GHz. In terms of memory, the laptop is equipped with 8 GB of RAM. The operating system utilized for these simulations is Windows 10, 64 bits. This configuration provides the necessary computational power and resources to conduct the simulations effectively, ensuring reliable and accurate results in the evaluation of the molecular communication system.

To facilitate the analysis, we initially introduce a set of assumptions that provide a convenient framework for our study. These assumptions serve as foundational principles upon which our subsequent evaluations and analyses. By establishing these assumptions, we aim to simplify the complexity of the problem and enable a more structured approach to our investigation.

1. In our system, we consider the transmitter to be a singular point source of molecules positioned at the origin. Furthermore, we assume that the transmitter is exclusively responsible for emitting these molecules. This assumption allows us to concentrate solely on the behavior and characteristics of the molecules originating from this centralized source.
2. Molecules are treated as immutable entities, preserving their identity without undergoing any changes or disappearing during their propagation.
3. After a molecule is released from the transmitter, we consider it to remain independent and assume that the molecule remains completely non-interacting with the transmitter. This assumption implies the absence of feedback or re-absorption mechanisms between the transmitter and the released molecules. By adopting this assumption, we can isolate the molecules' behavior and effects as they propagate and interact with the surrounding environment.
4. The receiver is defined as a spherical area that does not encompass the origin point.

System parameters considered in this simulation are given in Table 1.

Table 1. Simulation Parameters

Sr No	Parameter	Symbol	Value
1	Number of transmitting nodes	N_{tx}	1
2	Number of receiving nodes	N_{rx}	1
3	Transmitting node coordinates		(0,0,0)
4	Receiving node coordinates		(x,y,z)
5	Receiver Radius		R_{rx}
6	Number of emitted molecules	N	1000
7	Diffusion Coefficient	D	0.756 μm^2/Sec

Different steps involved in the simulation are as follows:

- **Transmitter**
  - Initial coordinates for the molecules located at the source side within the communication system are generated. These coordinates serve as the starting positions for the particles before they undergo diffusion and propagate through the system.
  - Randomly 'θ' and 'ϕ' values are generated.
  - Corresponding Cartesian coordinates (x, y, z) for the molecules are generated using the Equations (1), (2) and (3).

$$X = sin(\varphi) * cos(\theta) \quad (1)$$

$$Y = sin\ (\varphi) * sin\ (\theta) \tag{2}$$

$$Z = cos\ (\varphi) \tag{3}$$

here 'ϕ' represents the polar angle, which specifies the angle of rotation from the positive z-axis toward the positive y-axis. It ranges from 0 to π, covering half of a sphere. 'θ' represents the azimuth angle, which specifies the angle of rotation around the z-axis. It ranges from 0 to 2π, covering a full circle.

- **Channel Model and Propagation:** The subsequent step involves the characterization of how molecules propagate within a fluid medium.
  - The movement of an individual molecule within a unit of time can be depicted as a random variable (X) that adheres to a normal distribution.
  - Mathematically, the displacement of the molecule (X) can be represented as given in the Equation (4).

$$X = N(\mu, \sigma 2) \tag{4}$$

The normal distribution is defined by its mean (μ) and standard deviation (σ). The mean indicates the average displacement of the molecule, while the standard deviation dictates the extent of spread or variability in displacement values. We assume that molecules reach the receiver via diffusion, characterized by three-dimensional Brownian motion.

- – Let (X_0, Y_0, Z_0) represent the initial position of the molecule in three dimensions.
  – Thus, the molecule coordinates ($Xm_{(t)}$, $Ym_{(t)}$, and $Zm_{(t)}$) at time t can be updated at the time instant (t + Δt), for small Δt as,

$$X_m\ (t + \triangle t) = X_m\ (t) + X_1\sqrt{2D\triangle t} \tag{5}$$

$$Y_m\ (t + \triangle t) = Y_m\ (t) + Y_1\sqrt{2D\triangle t} \tag{6}$$

$$Z_m\ (t + \triangle t) = Z_m\ (t) + Z_1\sqrt{2D\triangle t} \tag{7}$$

Where X_1, X_2, and X_3 are Gaussian independent random variables, with mean $\mu = 0$ and variance σ^2. The variance' σ' is given by the Equation (8),

$$\sigma = \sqrt{2D\triangle T} \tag{8}$$

In the above expression, D represents the diffusion coefficient and ΔT represents the time interval. The time interval (ΔT) represents the duration over which the displacement is measured. The diffusion coefficient (D) characterizes the speed at which the molecule spreads in the environment. It is a measure of how quickly the molecule moves and diffuses through the medium. The formula gives the Diffusion coefficient,

$$D = \frac{4K_bT}{6\pi\eta R_H} \tag{9}$$

Where, K_b=1.38*10^{-23} J/K

T= Temperature in Kelvin

η= Viscosity of the fluid

R_H = Radius of propagating molecules

As per the Central Limit Theorem, the aggregation of numerous independent random variables tends to conform to a Gaussian or normal distribution, irrespective of the distributions of the individual variables.

- **Receiver**

The position of the receiver can be represented as a three-dimensional vector:

Receiver Position = (Receiver_x_value, Receiver_y_value, Receiver_z_value) This equation represents the coordinates of the receiver in the three-dimensional space,

where, Receiver_x_value represents the x-coordinate, Receiver_y_value represents the y-coordinate, Receiver_z_value represents the z-coordinate.

Surface Area: Surface area defines the total area of the outer surface of a three-dimensional object. We assume the receiver to be a sphere, and we calculate the surface area of a sphere using the formula:

$$Surface\ Area = 4 \times \pi \times R_{rx}^2 \tag{10}$$

Where R_{rx} denotes the radius of the sphere. The surface area of the receiver determines the area over which the molecules reach the receiver within a specified radius. In the subsequent step, the detection of molecule arrival at the receiver's end leads to the implementation of a destruction criterion. For each molecule, the analysis involves a comparison of its present coordinates with the receiver's established position and radius. The following conditions describe this comparison: The current coordinates of the molecule as (Xm, Ym, Zm), and the position of the receiver at (X_r, Y_r, Z_r). The receiver radius is denoted as R_{rx}. The molecule is considered received if it satisfies the conditions:

$$\sqrt{(X_m - X_r)^2 + (Y - Y_r)^2 + (Z_m - Z_r)^2} \leq R_{rx} \tag{11}$$

- **System Performance**
  - Then we calculate throughput, the rate at which the receiver successfully receives molecules, by counting the molecules reaching the receiver's range per unit time.
  - Finally, we calculate dynamic efficiency by dividing the molecules reaching the receiver by the total number of sent molecules. Dynamic efficiency provides an indication of how efficiently the receiver captures molecules based on given conditions.

Figure 2 summarizes the steps discussed in the above section.

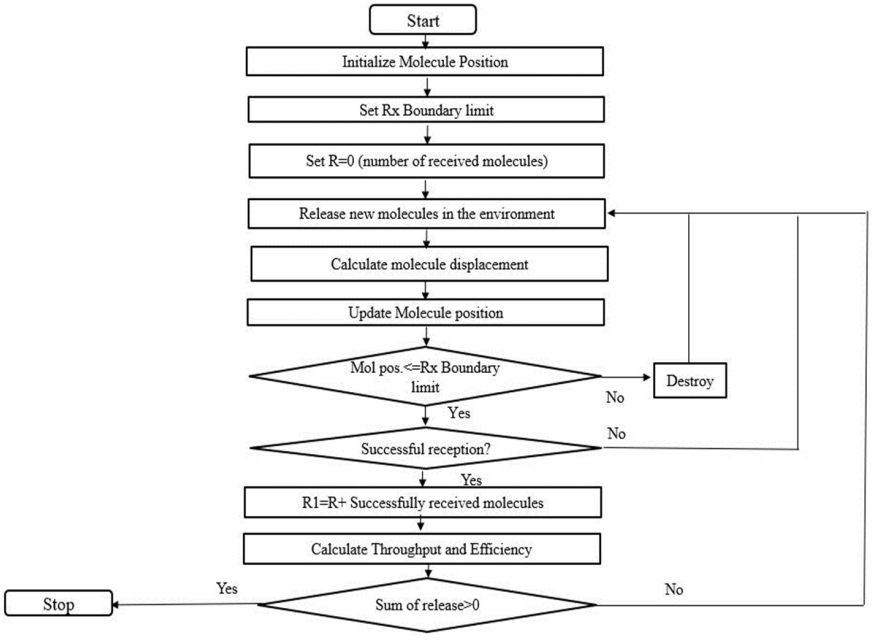

Fig 2. Flowchart of Molecular diffusion-reception process and throughput and efficiency calculation

3 Results and Discussion

We visualize the displacement of molecules in a three-dimensional space using a scatter plot. The x, y, and z coordinates of the molecules are represented in the plot as shown in Figure 3 **(a)**.

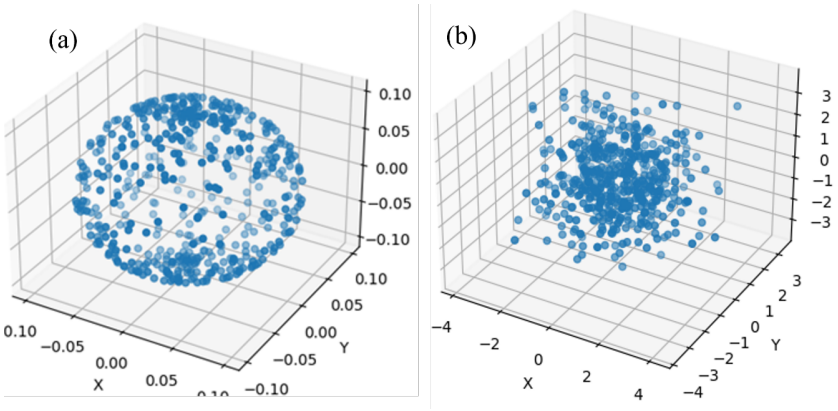

Fig 3. a) The generation of particles at source (b) Displacement of molecules

The displacement of molecules characterized by the wiener process is shown in Figure 3**(b).**

As shown in Figure 4**(a)**, as the molecule radius increases, the diffusion of larger molecules becomes slower compared to smaller molecules. This leads to longer diffusion times and limited propagation distances. Consequently, the effective concentration of signaling molecules at the receiver decreases, resulting in a reduced reception rate and, ultimately, decreased throughput. A larger molecule radius results in a shorter diffusion range and a limited coverage area. As the molecules diffuse, their effective concentration diminishes, and the area in which they can be successfully received becomes smaller. This restricts the communication range and limits the volume in which the receiver can reliably detect the molecules. As a result, the system's overall throughput and dynamic efficiency are reduced. The R^2 value for the parabolic curve of order 3 is 0.9686 which shows a good fit.

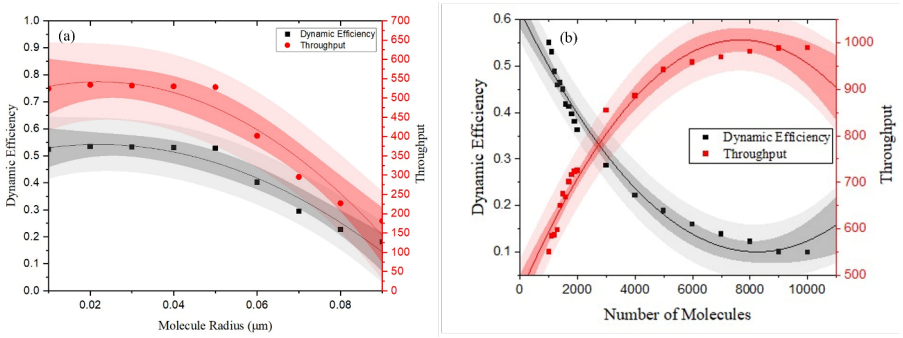

Fig 4. (a) Molecule Radius Vs Throughput and Dynamic Efficiency, (b) Number of sent molecules Vs Throughput and Dynamic Efficiency

As shown in Figure 4**(b)**, with a rise in the transmission rate, a greater quantity of molecules is diffused into the medium, thereby leading to an increased availability of molecules for the reception. The initial rise in the quantity of transmitted molecules correlates with an increase in the count of successfully received molecules, consequently enhancing the throughput. The relationship holds up to a certain point. Molecular communication channels have a limited capacity to carry information due to various factors such as diffusion limitations, interference, and noise. As the transmission rate increases, the channel's capacity is gradually approached, and at some point, it becomes saturated. Consequently, the channel reaches a point where it cannot accommodate a substantial rise in transmitted molecules, leading to decreased returns in throughput and dynamic efficiency as shown in Figure 4 **(b)**. The R^2 value for parabolic curve of order 2 is 0.99 which shows excellent fit.

As shown in Figure 5**(a)** as the diffusion rate increases, throughput and dynamic efficiency increases initially and then decreases. When the diffusion rate increases, molecules disperse more rapidly, covering larger distances in each amount of time. This expanded coverage allows more molecules to reach the receiver, resulting in an increased reception rate and improved throughput. The faster diffusion enables more efficient transport of signaling molecules, enhancing the overall performance of the communication system. The R^2 value for parabolic curve of order 3 is 0.99 which shows excellent fit.

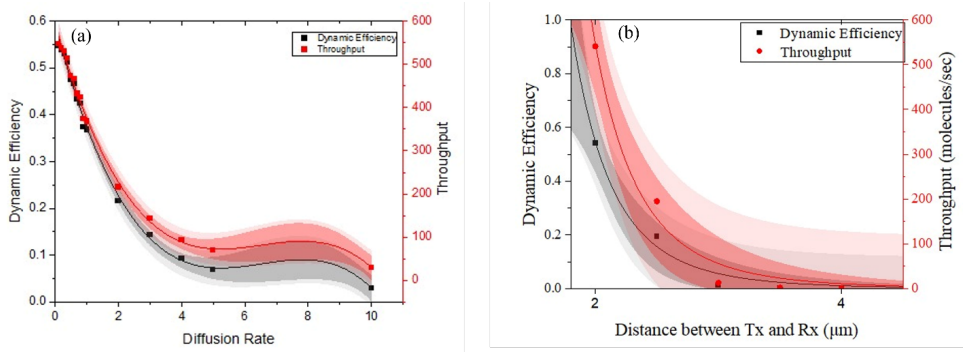

Fig 5. Diffusion Rate Vs Throughput and Dynamic Efficiency, (b) Distance between transmitter and receiver Vs Throughput and Dynamic Efficiency

With the rising gap between the transmitter and receiver, throughput and dynamic efficiency decrease as shown in Figure 5**(b)** because the communication channel encompasses a larger volume. This larger volume allows more molecules to be transmitted, leading to an initial reception. However, as the distance continues to increase, there comes a point where the signal strength of the transmitted molecules decreases with distance. As the molecules diffuse and propagate over a longer distance, their concentration decreases, resulting in a decrease in throughput and efficiency. The R^2 value for parabolic curve of order 3 is 0.98 which shows excellent fit.

4 Conclusion

This study emphasizes the complex interaction of multiple factors in the functioning of a molecular communication system. The optimal range for the receiver, the importance of diffusion rate, and the trade-off between molecule radius, transmission rate, and performance are all crucial considerations when designing and optimizing molecular communication systems. The study found that enhanced transmission rates result in a trade-off between throughput and efficiency. However, large molecule radius and increased distance between transmitter and receiver negatively impact both metrics. As the molecules diffuse and propagate longer distances, their concentration decreases, decreasing throughput and efficiency.

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