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Research Article

Modeling Channel Dynamics in Molecular Communication Systems

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ABSTRACT

Molecular Communication (MC) is a field that merges concepts from biology, chemistry, and information theory to enable information transfer using molecular signals. This work introduces a mathematical model for MC systems to deepen the understanding of key principles and improve nanoscale system design and optimization. The model addresses essential aspects, including molecular diffusion, advection, degradation, and channel impulse response in bounded environments. It investigates the effects of advection, where fluid flow influences concentration gradients and degradation processes, which impact signal robustness and duration. Both bounded and unbounded environments are analyzed to understand the dynamics of molecular concentration, with a focus on molecular confinement and channel conditions. Additionally, the study derives a channel impulse response equation essential for evaluating system performance. Simulation results offer insights into molecular concentration behaviors, advancing the understanding of MC systems.

Keywords: Molecular Communication, Diffusion, Channel Impulse Response, Advection.

1. Introduction

In today's world, communication plays a fundamental role in human interaction, facilitating the exchange of information across diverse mediums and vast distances. However, as technology advances and explores new frontiers, conventional means of communication encounter limitations, particularly when dealing with communication at the nanoscale. MC, a flourishing interdisciplinary field situated at the confluence of biology, chemistry, and information theory, presents a revolutionary approach to address these challenges. It focuses on the communication of information through the exchange of molecules, offering a unique perspective on communication systems operating at the nanoscale. This emerging field has garnered significant attention due to its potential applications in a wide array of domains, including medicine, environmental monitoring, and nanotechnology. MC systems leverage the inherent properties of molecules to transmit data, opening doors to innovative solutions for targeted drug delivery in healthcare, pollution detection in the environment, and enhanced control at the nanoscale in various technological applications.

This work provides a deeper understanding of MC by presenting a comprehensive mathematical model. Our aim is twofold: first, to explain the underlying principles and mechanisms governing MC, and second, to facilitate the design and optimization of communication systems that operate within this unique paradigm.

In this endeavor, the details of molecular diffusion, advection, degradation, and the characteristics of channel impulse response are considered. Furthermore, the impact of various channel conditions, such as diffusion, advection, and degradation, on the concentration of molecules received at different time intervals are considered. This investigation serves as a cornerstone in understanding the factors influencing the performance of MC systems.

Physical Principles in MC are described as follows:

1.1. Diffusion

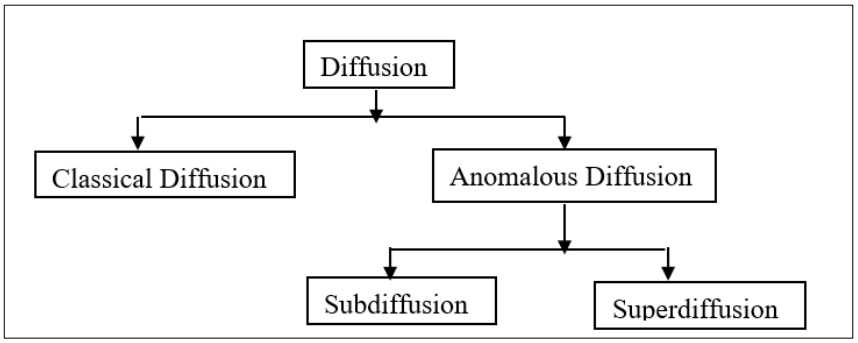

Figure 1: Classification of diffusion

1.1.1. Classical Diffusion

In a fluid environment, whether liquid or gas, molecules undergo constant motion due to thermal energy, causing them to collide with surrounding particles. This movement is entirely unpredictable and lacks a fixed direction, a phenomenon known as Brownian motion or random walk.

Let di(t) = [x, y, z] represent the location of i_{th} particle at time t. Consequently, the random walk is described as [1]

$$d_i(\mathrm{t} + \Delta\mathrm{t}) = d_i(\mathrm{t}) + \mathrm{N}(0, 2\mathrm{D}\Delta\mathrm{t}\,\mathrm{I}) \quad (1)$$

Here, Δt represents time step size, while D denotes the diffusion coefficient, measured in [m^2/sec]. N (μ, Σ) refers to a Gaussian random variable with a mean vector μ and covariance matrix Σ. The vector 0 consists entirely of zeros, and I represent the identity matrix. This coefficient is influenced by both environmental conditions and the particle's shape and size. For spherical particles, it can be derived using the Einstein relation [2].

$$D = \frac{K_B T}{6\pi\eta R} \quad (2)$$

where $K_B = 1.38 \times 10^{-23}$ JK^{-1} is Boltzmann's constant, T is Temperature in kelvin, η is (dynamic) viscosity of the fluid, and R is the radius of the particle.

1.1.2. Anomalous Diffusion

Anomalous diffusion, sometimes referred to as non-classical or sub-diffusion, describes a distinct type of random motion observed in various physical and biological systems. Anomalous diffusion follows a scaling behavior,

$$MSD \propto D\Delta t$$

In anomalous diffusion, the MSD follows a nonlinear relation, i.e.,

$$MSD \propto D\Delta t^{\gamma}, \text{ where } \gamma \neq 1.$$

There are two main types of anomalous diffusion:

1.1.2.1. Subdiffusion

In subdiffusion, particles exhibit slow movement compared to classical diffusion. This occurs when γ < 1 and

is often used in modeling biological cell diffusion, where organelles create obstacles that prevent ideal free diffusion [3]. In such cases, the mean squared displacement (MSD) increases at a slower rate than a linear function of time.

1.1.2.1 Superdiffusion

In superdiffusion, particles move faster than expected for classical diffusion. Superdiffusion takes place when $\gamma > 1$ describes active cellular transport processes [4]. The MSD of particles grows more quickly than linearly with time. Super diffusion can be observed in systems with complex interactions, such as turbulent flows, active matter systems, or in some biological processes like the motion of certain molecules within cells.

1.2 Boundary Conditions

1.2.1 Diffusion in an Infinite 3-D Space

The random motion of molecules driven by diffusion, as described in equation (1), results in the second law of diffusion over time and space.

$$\frac{\partial c(d,t)}{dt} = D\nabla^2 c(d,t) \quad (3)$$

The eqn. (3) for initial and boundary conditions (ICs and BCs)

$$\text{IC1} : c(do, t \rightarrow to) = N\delta(d - do) \quad (4)$$

$$\text{BC1}: c(d \rightarrow \infty, t) = 0 \quad (5)$$

where $\delta(d) = \delta(x)\,\delta(y)\,\delta(z)$ And $\delta(\cdot)$ is the Dirac delta function.

Solving (3) with IC1 and B1 yields [1]

$$N(d,t) = \frac{N}{(4\pi D(t-to))^{3/2}} \exp\left(-\frac{|d-d0|^2}{4D(t-to)}\right) \quad (6)$$

1.2.2 Diffusion in a bounded 3-D Environment

For cylindrical coordinates represented as $d = [\rho, \phi, z]$, the parameters are constrained with $0 \le \rho \le r_c$, $0 \le \phi \le 2\pi$ $-\infty < z < +\infty$, where r_c defines circular cross-section radius of bounded channel.

At the initial release of time t_o, the molecules are evenly dispersed across the cross-section at $z = z_o$.

Therefore, IC and BCs are:

$$\text{IC2} : c(do = [\rho, \phi, z], t \rightarrow to)\frac{N}{\pi rc2}\delta(z - zo) \quad (7)$$

$$BC2 : \partial c(d,t) \,/\, \partial\rho \mid \rho = rc = 0 \quad (8)$$

$$BC3 : c(d = [\rho, \phi, z \rightarrow \pm\infty], t) = 0 \quad (9)$$

Here, BC2 ensures that molecules reflect off the wall, assuming a fully reflective surface. By solving equation (3) with IC2, BC2, and BC3, the following result is obtained [4].

$$N(d,t) = \frac{N}{\pi rc^2\sqrt{(4\pi D(t-to))^{3/2}}} \exp\left(-\frac{|d-d0|^2}{4D(t-to)}\right) \quad \rho \le r_c \quad (10)$$

1.3 Advection

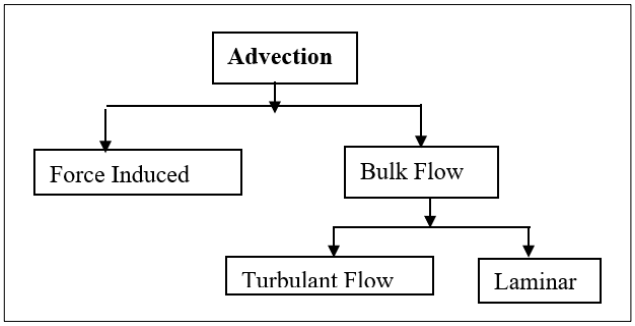

Figure 2: Classification of Advection

In addition to diffusion, this advection represents an even more critical process in transporting particles of solute particles dissolved in a fluid. Generally, the movement by advection can be expressed as v (d, t). The i_{th} particle at the $(t + \Delta_t)$ given as,

$$di(t + \Delta t) = di(t) + v(di(t), t)\Delta \qquad (11)$$

Advection transport can occur through various physical mechanisms, broadly classified into force-induced drift and bulk flow[5], [6].

1.3.1 Force-induced drift

The movement driven by advection can originate from external forces impacting the particles rather than the fluid encompassing them. Such external forces can be mathematically represented by a force vector F(d, t). When applied force is relatively small, the velocity vector can be derived using Stokes' law [6].

$$\text{v(d, t)} = \frac{F(d,t)}{\zeta} \qquad (12)$$

Here, ζ friction coefficient, given as $\zeta D = kBT$

Thus, using Equation (2), ζ can be expressed as, $\zeta = 6\pi\eta R$.

1.3.2 Bulk flow

When particle movement is driven by fluid motion, the resulting transport is known as advection or flow. This phenomenon occurs in various molecular communication (MC) environments, including blood vessels and microfluidic channels [7]. The velocity varies across space in the presence of boundaries or obstacles. For instance, in a duct, fluid flow is generally fastest at the center and slows near the boundaries due to friction.

Flow is generally classified as turbulent flow and laminar flow. Turbulent flow occurs when the velocity fluctuates unpredictably over space and/or time, often due to uneven surfaces or elevated velocities. In contrast, laminar flow is smooth and lacks such turbulence. In a confined environment, the Reynolds number distinguishes between laminar and turbulent [8]

$$\text{Reynolds number} = \frac{\text{deff} \cdot \text{v}_{eff}}{v} \qquad (13)$$

where ν is the kinematic viscosity [m^2/s] of the fluid, with a d_{eff} effective length and v_{eff} an effective velocity.

In microfluidic environments, the Reynolds number is typically around 10, indicating that laminar flow [6]. In blood vessels, the Reynolds number remains below 500, meaning flow is generally laminar [9]. However, in larger arteries, such as the aorta (the body's largest artery), the Reynolds number typically ranges from 3400 to 4500, resulting in turbulent blood flow. [10].

Thus, the advection equation or continuity equation is represented as,

$$\frac{\partial N(d,t)}{dt} = -\nabla \cdot (\text{v (d, t)c(d, t)} \qquad (14)$$

1.4 Advection–Diffusion

In applications such as drug delivery via the capillary networks [11], there is a combined effect of both advection-diffusion. The advection-diffusion equation is given by,

$$\frac{\partial c(d,t)}{\partial t} = D\nabla^2 c(d,t) - \nabla . v(d,t)c(d,t) \qquad (15)$$

Solution of the above equation in an unbounded environment:

For a three-dimensional unbounded environment with IC1 from (4), BC1 from (5), $N(d,t) = \frac{N}{(4\pi D(t-t0))^{3/2}} *$

$$e^{\left(-\frac{|d-(t-to)v-d0|^2}{4D(t-to)}\right)} \quad t>to \qquad (16)$$

1.5 Chemical Reactions

Another significant factor influencing the transmission of molecules in MC is the occurrence of chemical reactions. These reactions can naturally take place within MC environments, necessitating their careful consideration in the design of communication strategies, Figure (3) depicts the classification of chemical reactions.

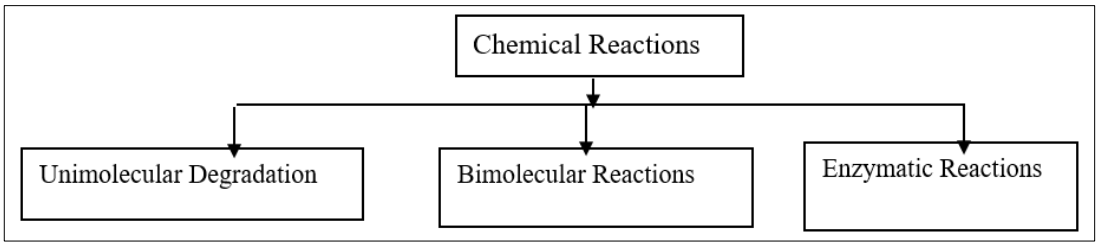

Figure 3: Classification of Chemical Reactions

1.5.1 Unimolecular Reactions

This process represents the degradation of a specific molecule, such as type A, into another molecule, denoted as φ, which is not relevant to the current communication analysis. Unimolecular degradation is frequently employed as an initial approximation for more complex reactions.

1.5.2 Bimolecular Reactions

Certain results involve two initial chemical species, such as P and Q, leading to the creation of molecules like C. For instance, signaling molecule interactions that activate ligand receptors have been modeled using a second-order bimolecular reaction.

1.5.3 Enzymatic Reactions

In certain situations, natural degradation may occur too slowly relative to the required communication time scale. To expedite the reaction process, enzymes can be introduced as catalysts.

1.5.4 Advection–Reaction–Diffusion Equation

Considering the combined influence of diffusion, drift, and reactions, advection-reaction-diffusion equation is expressed as

$$N(d,t) = \frac{N}{(4\pi D(t-t0))^{3/2}} e^{\left(-(k(t-to))-\frac{||d-(t-t0)v-d0||^2}{4D(t-t0)}\right)} \qquad (17)$$

1.6 Channel Impulse Response

Channel Impulse Response (CIR) is a mathematical representation that characterizes how the channel reacts to an impulse. It illustrates the channel's behavior over time and helps predict signal distortion as it propagates through the medium.

2. Literature Review

MC is an evolving paradigm that facilitates nanoscale devices to exchange information by mimicking biological communication processes. It utilizes molecules as carriers to transmit data between nanomachines over short distances, ranging from adjacent nanomachines to a few tens of micrometers. In this communication framework, a sender releases molecules into the surrounding environment, which then propagate toward a designated receiver. MC presents vast potential across various domains, including biomedical applications, environmental monitoring, nanoscale sensor networks, and targeted drug delivery systems.

Atakan et al. [15] explored an information-theoretic perspective on MC, addressing challenges in controlled molecular transmission. They proposed a ligand-receptor binding model and proposed an expression to determine the molecular channel's capacity. Their findings indicate that optimizing MC parameters—such as temperature, molecule concentration, distance between devices, and emission duration—can significantly enhance channel capacity. Similarly, Liu et al. [16] introduced an MC model inspired by cellular signaling, where second messengers facilitate molecular exchange between senders and receivers. By leveraging cellular pathway networking, the study identified self-organizing mechanisms applicable to dynamic networks.

Eckford [17] conceptualized MC within an information-theoretic framework, formulating mathematical models to analyze communication channels. The study provided upper and lower bounds on mutual information, balancing computational complexity with accuracy. Moore et al. [18] designed an in vitro MC system where a sender encodes data onto molecules that undergo chemical reactions upon reaching a receiver. Their work employed simulations to evaluate information transmission probabilities and optimize MC system design. Additionally, Moore et al. [19] examined distance estimation between a transmitter and receiver nanomachine via molecular diffusion, considering different signal patterns such as single spikes, fixed-rate transmission, and wave-based signaling.

Atakan et al. [20] also introduced a stochastic model of biochemical molecular reactions, defining a deterministic capacity expression for various molecular communication channels, including point-to-point, broadcast, and multiple-access scenarios. Kadloor et al. [21] simplified mutual information calculations, proposing upper-bound estimates for information transfer in fluid mediums with drift, though their assumptions limit general applicability.

Farsad et al. [22] developed a mathematical model for MC systems using active transport propagation, demonstrating close agreement between estimated and simulated information rates for short communication intervals. Chou et al. [23] proposed the reaction-diffusion equation, modeling molecular transmitters as time-series molecular counts and incorporating Markov processes to account for diffusion and chemical reactions. Noel et al. [24] applied dimensional analysis to assess diffusive MC systems utilizing enzymes to mitigate intersymbol interference, establishing a lower bound for molecule detection at the receiver.

Lee et al. [25] introduced a machine-learning approach that models multiple-input multiple-output (MIMO) channels, confirming the method's effectiveness through extensive numerical studies. Chouhan et al. [26] derived an expression aimed at the expected hitting rate in a three-dimensional unbounded MC channel, identifying an optimal decision threshold that minimizes error probability while maximizing information transfer. Fatih et al. [27] analyzed the impulse response of channels,]showing how diffusion coefficients impact communication performance. Additionally, Noel et al. [24] derived impulse response functions for MC scenarios featuring spherical transmitters and passive or absorbing receivers, validating the accuracy of the point transmitter assumption. Lastly, Ferrari et al. [29] developed a model for the impulse response to enhance the understanding of molecular diffusion dynamics in detail.

These studies collectively advance the understanding of molecular communication, refining theoretical models and experimental approaches to enhance MC system design and efficiency across various applications.

3. System Model

Figure 1 depicts an MC system that consists of a point transmitter, a spherical receiver with a radius of a_c, and a bounded circular channel. Considering molecular diffusion is influenced by

time-dependent flow v(t) and degradation effects.

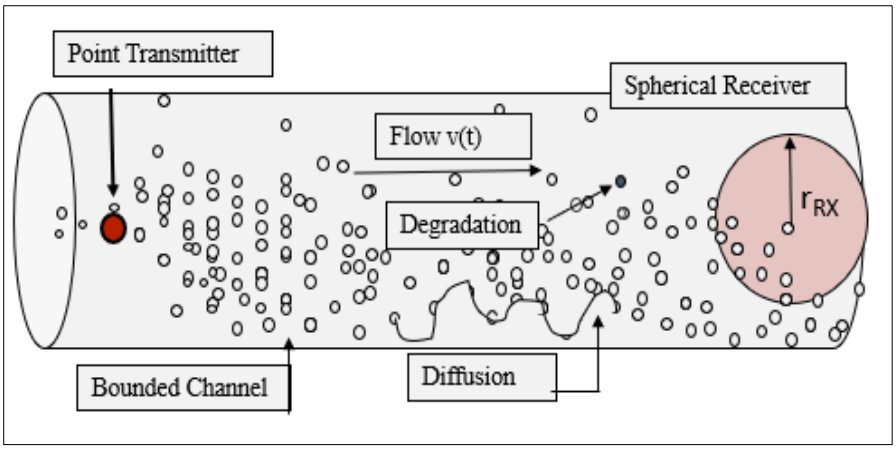

Figure 4 The proposed system model

The performance of the system is validated by observing concentration in bounded and unbounded conditions.

Point transmitters offer several advantages:

- Spatial Precision: Point transmitters allow for highly precise spatial targeting, enabling communication with specific receiver cells or receptors in a localized area. This precise targeting is crucial for ensuring that the intended recipient receives the message accurately.
- Low Energy Consumption: Compared to other forms of communication, MC using point transmitters typically requires less energy consumption.

Spherical Receiver offers several advantages:

- Omni-directional Reception: Spherical receivers have the advantage of being able to receive signals from all directions, allowing them to capture molecular signals coming from any point source.
- Scalability: Spherical receivers can be scaled to different sizes, making them adaptable to various biological contexts and applications.

4. Methodology

The molecular concentration dynamics in a bounded medium were analyzed using simulations implemented in the Python programming language. The concentration N(d, t) (in molecules/m³) was observed at different distances d over time. Concentration levels were examined at distances. Python-based numerical simulations were conducted to model molecular diffusion and reaction kinetics. The simulations incorporated variations in receiver radius a_c, flow velocity (v), and reaction rate constant (k).

In the latter part of the study, the channel impulse response was examined for various receiver radii a_c at different time instances.

4.1 Simulation Parameters

TABLE 7.1 SIMULATION PARAMETERS

Sr No	Parameter Name	Value
1	Tx Node	1
2	Rx Node	1
3	Distance between Tx and Rx (d)	(100,200,300,400,500) nm

4	Bounded Channel Radius (ac)	(1,2,3,4,5) nm
5	Degradation Rate (k)	(1,2)*10^4(1/sec)
6	Diffusion Coefficient(D)	4.5 × 10^{-10} m^2/s
7	Number of emitted molecules(N)	10000

4.2 CIR Derivation

The Channel Impulse Response (CIR) helps in predicting signal distortion during transmission.

It starts with Fick's law of diffusion and applies appropriate boundary conditions to derive the channel impulse response. The derivation involves solving the diffusion equation in spherical coordinates and applying boundary conditions. Here's a step-by-step derivation:

Fick's first law of diffusion relates the flux of molecules to the concentration gradient [30]:

$$J = -D\nabla C \quad (18)$$

Where J - flux of molecules, D - diffusion coefficient, C - concentration of molecules, ∇ - gradient operator, r - radial distance from the transmitter (point source) to any point in the medium, θ - polar angle. Φ - azimuthal angle.

The diffusion equation is derived by considering the change in concentration concerning time.

$$\frac{\partial C}{\partial t} = \boldsymbol{D\nabla^2 C} \quad (19)$$

Now, to solve this equation for concentration $C(r,t)$, a function of both time t and radial distance r. To do this, assume that the only source of molecules is at the origin (transmitter) at r = 0. So, consider an initial condition:

$$\boldsymbol{C(r,0) = \delta(r)} \quad (20)$$

Where $\delta(r)$ Is the Dirac delta function representing an instantaneous release of molecules at the transmitter location at t = 0?

Applying Spherical Symmetry

Due to the spherical symmetry of the problem (since having a spherical receiver), assume spherical C is only a function of r and t :

$$C(r,t) = R(r) \times T(t) \quad (21)$$

Substituting this into the time-dependent diffusion equation:

$$R(r) * \frac{\partial T}{\partial t} = DT(t)\nabla^2 R(r) \quad (22)$$

Separation of Variables

Separate the variables R and T and set them equal to constants:

$$\frac{1}{R(r)}\nabla^2 R(r) = \frac{1}{D}\frac{1}{T(t)}\frac{\partial T}{\partial t} = -\lambda^2 \quad (23)$$

This leads to two separate equations: One for T(t) and One for R(r)

Time-Dependent Part: The time-dependent part T(t) has a simple solution:

$$\frac{\partial T}{T(t)} = -\lambda^2 D dt \qquad (24)$$

Integrating both sides

$$\int \frac{\partial T}{T(t)} = \int -\lambda^2 D\, dt \qquad (25)$$

$$\ln T(t) = -\lambda^2 D \int dt \qquad (26)$$

$$\ln T(t) = -\lambda^2 Dt + C \qquad (27)$$

At t=0,

$$\ln T(0) = 0 + C \qquad (28)$$

$$C = \ln T(0) \qquad (29)$$

Substituting eqn (29) in eqn (27)

$$\ln T(t) - \ln T(0) = -\lambda^2 Dt \qquad (30)$$

$$\ln \frac{T(t)}{T(0)} = -\lambda^2 Dt \qquad (31)$$

$$\frac{T(t)}{T(0)} = e^{(-\lambda^2\ Dt)} \qquad (32)$$

$$T(t) = T(0)e^{(-\lambda^2 Dt)} \qquad (33)$$

Radial Part

The radial part R(r) can be solved using spherical Bessel functions, and the general solution is:

1. Spherical Bessel Functions:

Spherical Bessel functions are a set of special functions used in solving problems with spherical symmetry. They are denoted by $Jn(x) and\ yn(x)$, where n is a non-negative integer, and x is the argument.

Jn(x) is the regular spherical Bessel function of the first kind.

$yn(x)$ It is the irregular spherical Bessel function of the second kind.

These functions arise naturally when solving partial differential equations in spherical coordinates, such as the diffusion equation in our case.

2. The General Solution for R(r):

In the context of our problem, the radial part R(r) is expressed as a combination of spherical Bessel functions:

$$R(r) = A.\frac{\sin(\lambda r)}{r} + B\frac{\cos(\lambda r)}{r} \qquad (34)$$

Here's what each term represents:

- A and B are constants that depend on the boundary conditions and eigenvalues.
- λ is one of the eigenvalues
- The first term $A.\frac{\sin(\lambda r)}{r}$ corresponds to the regular spherical Bessel function j1(λr)

The second term $B\frac{\cos(\lambda r)}{r}$ corresponds to the irregular spherical Bessel function y1(λr)

Applying Boundary Conditions:

At r= $r_{Rx,}$ impose the condition of zero concentration :

$$R(r_{Rx}) = 0 \qquad (35)$$

This leads to a set of eigenvalues λn

Channel Impulse Response

The CIR is the product of time-dependent part T(t) and radial part R(r)

$$h(r,t) = T(t) * R(r) \qquad (36)$$

Substituting the solutions for T(t) and R(r) along with the eigenvalues λn, obtain the final expression for the channel impulse response. Moreover, this expression would be complex and involve summations over multiple eigenvalues, depending on the specific values of Rx and D.

7.4 Concentration of molecules in a bounded and unbounded medium

Fick's Second Law is given as.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad (37)$$

For constant Surface Concentration is Cs → Initial Concentration in homogeneous at x→∞ C=C0

→ x

The boundary conditions that solve above equation is

$$C(0,t) = Cs \qquad \text{at } t>0 \text{ (t slightly greater than 0)}$$

$$C(\infty,t) = C_0 \qquad \text{at } t>0$$

The IC is

$$C(x,0)= Co \qquad 0 \le x \le \infty$$

Using the above conditions, the solution is

$$\frac{C(x)-C0}{Cs-C0} = 1 - \text{erf}\left(\frac{x}{\sqrt{4Dt}}\right) \qquad (38)$$

Where erf is the error function given by

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-z^2}dz$$

Eqn (38) can be simplified for C_0=0

$$C(x,t)= Cs\left(1-\text{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right) \qquad (39)$$

Using the value of eqn (39) and putting

$$z = \frac{x}{\sqrt{4Dt}}$$

$$\text{Resultserf}(z) = \frac{2}{\sqrt{\pi}} \int_0^{\left(\frac{x}{\sqrt{4Dt}}\right)} e^{-\left(\frac{x}{\sqrt{4Dt}}\right)^2} d\left(\frac{x}{\sqrt{4Dt}}\right) \quad (40)$$

Where, $Cs = \frac{N}{\sqrt{4\pi Dt}}$ Is surface concentration.

N- total number of molecules/ area

Applying the similar mathematical calculations, get the solution for

i) Diffusion in an unbounded 3-D environment

With IC1: C (d_o, t ~~→ to~~) = $N\delta(d - do)$

BC1: C(d ~~→ ∞~~) = 0

$$C(d,t) = \frac{N}{\sqrt{4\pi D(t-to)}} \exp\left(-\frac{(d-d0)^2}{4D(t-to)}\right) \quad (41)$$

N- Number of molecules/area

It can be correlated with eqn. (41), which is the solution for Fick's second law used for doping concentration in a semiconductor material.

Similarly for

ii) Straight duct with impulsive release having an area of cross-section (πac^2) with cylindrical coordinates, d≡(ρ,ϕ,z)

IC2: C($d_{o \equiv [\rho,\phi,z]}$, t ~~→ 0~~) = $\frac{N}{\pi ac^2}\delta(z - z0)$

BC2: $\frac{\partial}{\partial t} C(d,t)|$ ρ=ac

BC3: C(d=[ρ, ϕ,z] ~~→ ∞~~, t)=0

Solution will be

$$C(d,t) = \frac{N}{\pi ac^2\sqrt{4\pi D(t-to)}} \exp\left(-\frac{(z-z0)^2}{4D(t-to)}\right) \quad (42)$$

Here, $\frac{N}{\pi ac^2}$ is number the of molecules /Area of cross section.

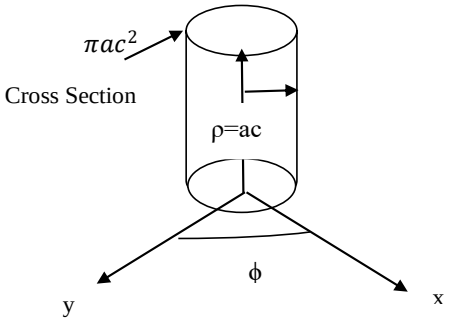

Fig. 7.1 Straight Duct

iii) Advection-Diffusion effect in straight duct with impulsive release having an area of cross-section (πac^2) with cylindrical coordinates, d≡(ρ,ϕ,z)

The combined effect of advection and diffusion [31] is given by

$$c(d,t) = \frac{N}{(4\pi D(t-t0))^{3/2}} e^{\left(-\frac{||d-(t-t0)v-d0||^2}{4D(t-t0)}\right)} \qquad (43)$$

The combined effect of both advection and diffusion in the bounded medium is characterized by the following equation obtained from eqn(43)

$$c(d,t) = \frac{N}{\pi ac^2(4\pi D(t-t0))^{3/2}} e^{\left(-\frac{||d-(t-t0)v-d0||^2}{4D(t-t0)}\right)} \qquad (44)$$

iv) Advection-Diffusion-Reaction effect in straight duct with impulsive release having an area of cross-section (πac^2) with cylindrical coordinates, d≡(ρ,ϕ,z)

For effective communication design, it is essential to consider their chemical reaction's impact. The interplay of advection, diffusion, and reaction is described by [31]

$$c(d,t) = \frac{N}{\pi ac^2\left(4\pi D(t-t0)\right)^{\frac{3}{2}}} e^{\left(-(k(t-to))-\frac{||d-(t-t0)v-d0||^2}{4D(t-t0)}\right)} \qquad (45)$$

From eqn (45), the combined effect of advection, diffusion, and reaction in the bounded medium is characterized by,

$$c(d,t) = \frac{N}{\pi ac^2\left(4\pi D(t-t0)\right)^{\frac{3}{2}}} e^{\left(-(k(t-to))-\frac{||d-(t-t0)v-d0||^2}{4D(t-t0)}\right)} \qquad (46)$$

5. Results

Fig 8 (a) depicts the Molecule concentration versus time at distances (100,200,300,400,500) nm for 10000 molecules released in an unbounded medium.

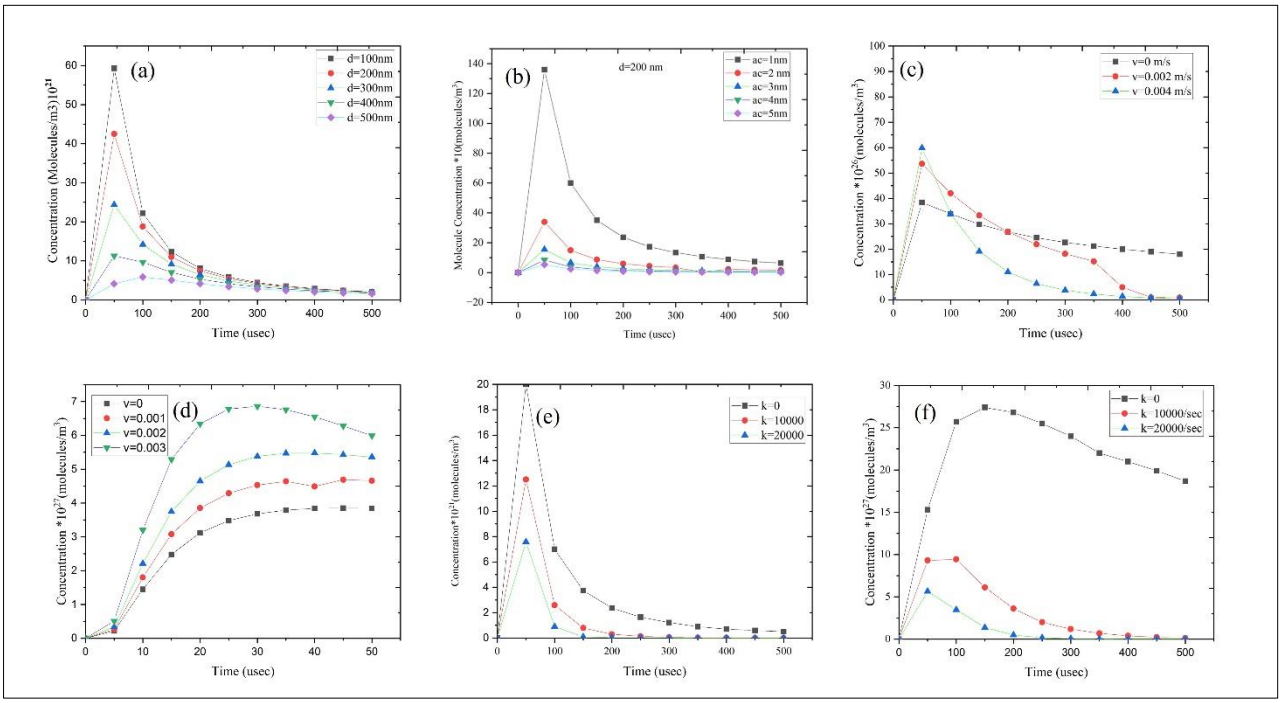

Fig (a) Molecular Concentration vs. time in unbounded medium (b) Molecular Concentration vs. time in bounded medium (c) Advection effect on Molecular Concentration for various velocities in bounded medium (d) Advection effect on Molecular Concentration for various velocities in bounded medium for time step (e) Advection degradation effect on Molecular Concentration for various velocities in an unbounded medium (f) Effect of advection degradation on molecular concentration in a bounded medium

Initially, concentration rises over time as molecules travel to reach point *d*. This is followed by a decline as molecules disperse. With increasing distance, the concentration peak diminishes due to greater distribution.

The second observation was done by observing the molecule concentration at different time instants in a bounded medium. The observation was made for different distances (300,400,500) nm.

Fig. 8. (b) depicts the molecular concentration at different time instants in the bounded medium. In this case, the influence of boundaries on the behavior of diffusing molecules is considered. Initially, concentration increases over time. This behavior is a consequence of the finite amount of time required for molecules to travel and reach point d. Moreover, this upward trend is followed by a subsequent decrease as the molecules gradually disperse. As the cross-section radius expands, the molecules detected are more compared to an unbounded medium. However, a larger cross-section radius results in a lower concentration peak, as the molecules spread over a wider area.

Figure 8 (c) and (d) illustrate the impact of advection on molecular concentration at different velocities within the bounded medium. With an increase in flow velocity, the concentration peak rises, and the peak appears earlier. This phenomenon primarily results from the flow direction aligning with the point where concentration is being evaluated.

Furthermore, increasing the velocity (v) has the effect of reducing the tail of concentration over time, which proves advantageous for mitigating Inter-Symbol Interference (ISI) in MC systems.

Fig 8. (e) depicts the advection degradation effect on Molecular Concentration for various velocities in the bounded and unbounded medium, respectively. The intensity of molecules in the bounded medium is greater than unbounded because of the influence of boundaries on the behavior of diffusing molecules. When the degradation rate increases, there is an undesired decrease in the concentration peak.

Nevertheless, there is a notable benefit as the concentration's tail, particularly for larger time values (t), diminishes at a swifter pace with higher degradation rates. This aspect proves advantageous for reducing Inter-Symbol Interference (ISI).

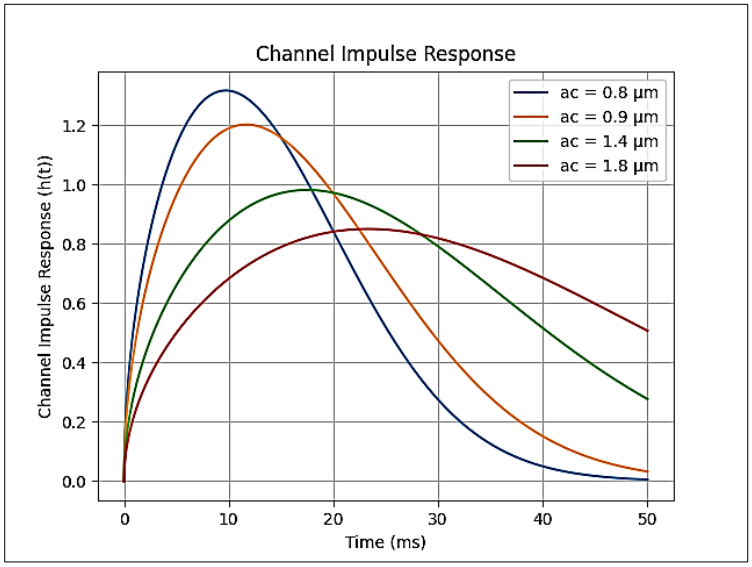

Fig. 9 Channel Impulse Response h(t) Vs Time

Fig 9 illustrates the CIR h(t) of a bounded circular channel. For each value of the duct radius, the CIR exhibits a distinct peak at an initial time and then gradually decays over time. Larger values of the duct radius result in wider and delayed peaks. Smaller values result in narrower and earlier peaks. This indicates that the duct radius has a significant impact on the timing and shape of the CIR.

6. Conclusion

This study has provided an analysis of fundamental principles governing MC systems, emphasizing the critical role of mathematical models in understanding the dynamics of communication at the nanoscale. By incorporating core aspects such as diffusion, advection, and degradation, the models presented in this study have demonstrated their efficacy in capturing the complex behavior of signaling molecules within the communication channel. Through analytical assessments and simulation outcomes, the influence of various parameters, including boundary conditions, flow velocity, and degradation rates, on molecule concentration profiles and channel impulse responses were explored. These investigations have not only deepened understanding of the complex interaction between environmental factors and communication performance but also have highlighted the significance of real system design in medical applications, ensuring reliable and efficient MC.

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