
MCvD WITH MULTIPLE TRANSMITTERS AND RECEIVERS

EE698U: INTRODUCTION TO MOLECULAR COMMUNICATION, SPRING 2022

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ABSTRACT

In this term paper, we aim to analytically study different systems involving molecular communication via diffusion (MCvD) with multiple transmitters and receivers. In particular, we first consider multiple transmitters and receivers distributed according to Poisson Point Processes in unrestricted 3D space. Next, we look at multiple transmitters and receivers placed in a duct-like channel, studying effects of advection in an attempt to apply this to real-life environments such as blood vessels. Finally, we briefly consider partially counting fully absorbing receiver and propose further directions unifying the presented analyses into a novel system.

1 Introduction

There has been a lot of research into analyzing distributed molecular communication systems with multiple transmitters and receivers. [1] considers such a distributed system, with point transmitters and passive spherical receivers placed at locations governed by a homogeneous Poisson point process (HPPP). The transmitters are also capable of emitting molecules asynchronously, which is again modeled by a PP. [2] considers a system with a single point transmitter at the origin and two spherical fully absorbing receivers located in 3D space and derives the channel response by fitting simulation data. [3] provides an approximate analytical expression for the same system.

[4] provides the expressions for the detection probabilities for any one of multiple fully absorbing spherical receivers with a single point transmitter at the origin. [5] extends the analysis of this system further by deriving the channel impulse response of each receiver. [6] calculates the hitting probabilities for each receiver in the system considered in [7] and further analyzes a SIMO system with the receivers placed in a Uniform Circular Array.

Vessel-like channels have been analyzed in many past works. [8] analyzes the performance of a molecular communication system based on advection-diffusion particle transport in a duct-like channel. [9] considers the use of mobile relays in a diffusion-advection flow channel. [10] derives the radial and axial distribution of the molecules in a microfluidic channel under Poiseuille flow. [11] proposes partially counting absorbing receivers, in which molecules that hit only a certain portion of the receiver's surface are counted as received information.

The paper is organized as follows: Section 2 presents the analysis for multiple transmitters and passive receivers placed according to PPPs in unrestricted 3D space. Section 3 attempts to apply techniques presented in [5] to extend the analysis in the previous section to fully absorbing receivers. Section 4 considers multiple transmitters in a duct-like channel, with both passive as well as fully absorbing receivers. Section 5 presents an analysis for partially counting fully absorbing receivers introduced in [11]. Section 6 concludes by presenting the takeaways and further directions for developing and analysing new systems.

2 Multiple Transmitters and Passive Receivers in 3D

In this section, we consider the model presented in [1].

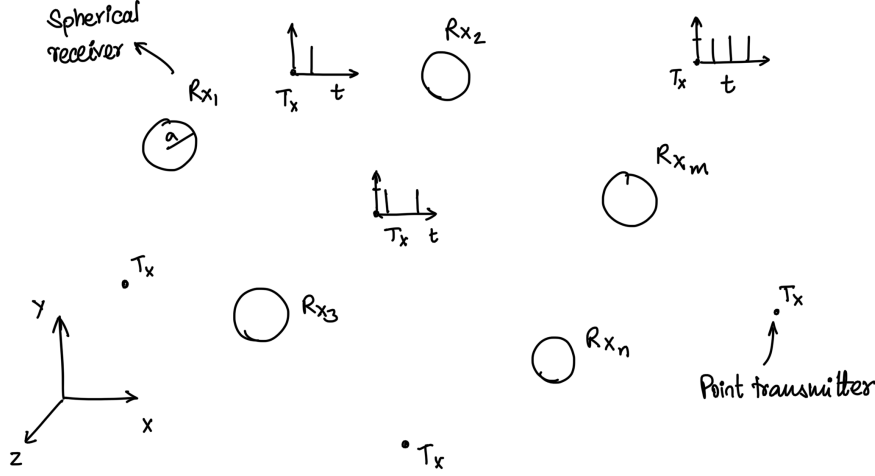


Figure 1: Multiple transmitters and receivers in 3D

2.1 System Model

Figure 1 provides a visualization of the considered system. The system model is described as follows:

- Transmitters and receivers are randomly placed in 3D space. The transmitters are simply points. The receivers are spheres of radius a .
- The positions of the centers of the receivers are determined by a homogeneous Poisson point process.
- The emission of molecules from the transmitters is asynchronous. It is controlled by independent time PPPs with the same intensity function that represent the propensity function of a chemical reaction.
- The medium is considered unbounded, where the molecules can diffuse with a constant diffusion coefficient D . The molecules do not undergo degradation.
- The receivers are passive.

2.2 System Analysis

2.2.1 Transmitter and Receiver Positions

The position of the n^{th} receiver x_n is a random variable belonging to a homogeneous Poisson Point Process $\Pi_{R_x} \in \mathcal{R}^3$ with intensity λ_{R_x} .

The position of the k^{th} transmitter x_k can be a random variable belonging to a homogeneous Poisson Point Process $\Pi_{T_x} \in \mathcal{R}^3$ with intensity λ_{T_x} . However, we note that there are infinite receivers in the same space. Since the receiver volume is not considered to be negligible, the space in which the transmitters can be placed is reduced significantly. Thus, the transmitter positions are actually determined by a Poisson Hole Process. We further approximate this as a homogeneous Poisson Point Process $\Pi_{T_x} \in \mathcal{R}^3$ with intensity λ_{T_x} . The derivation is presented below.

Consider a set $\mathcal{B} \in \mathcal{R}^3$. The expected number of points of a PPP that lie in the set \mathcal{B} is $|\mathcal{B}|\lambda$, where λ is the intensity of the PPP. Now, we consider the expected number of points due to a PHP Π_{T_x} induced by the PPP Π_{R_x} . We calculate this by considering a baseline PPP Π_1 of intensity λ_1 , and considering only those points that do not have any receiver centre within a radius of a , which is the radius of the receiver.

$$\begin{aligned}
 &= E \left[\sum_{x \in \Pi_1 \cap \mathcal{B}} \prod_{y \in \Pi_{R_x}} (1 - \mathbb{1}_{B(x,R)}(y)) \right] \\
 &= E_{\Pi_1} \left[\sum_{x \in \Pi_1 \cap \mathcal{B}} E_{\Pi_{R_x}} \left[\prod_{y \in \Pi_{R_x}} (1 - \mathbb{1}_{B(x,R)}(y)) \right] \right] \\
 &= E_{\Pi_1} \left[\sum_{x \in \Pi_1 \cap \mathcal{B}} \exp \left(- \int_{\mathcal{R}^3} \lambda_{R_x} \mathbb{1}_{B(x,R)}(y) dy \right) \right] \\
 &= E_{\Pi_1} \left[\sum_{x \in \Pi_1 \cap \mathcal{B}} \mathbb{1} \right] \exp \left(- \int_{\mathcal{R}^3} \lambda_{R_x} \mathbb{1}_{B(x,R)}(y) dy \right) \\
 &= |\mathcal{B}| \lambda_1 \exp \left(- \lambda_{R_x} \frac{4}{3} \pi a^3 \right) = |\mathcal{B}| \lambda_{T_x}
 \end{aligned}$$

Thus, $\lambda_{T_x} = \lambda_1 \exp \left(- \lambda_{R_x} \frac{4}{3} \pi a^3 \right)$ is the intensity of the equivalent PPP.

2.2.2 Transmitted Signal

The emissions of the k^{th} transmitter are determined by a time Poisson Point Process ϕ with non-homogeneous intensity $\rho(t)$. The points belonging to the time PP represent the time instants at which the transmitter releases a molecule. Hence, we can write the signal transmitted by the k^{th} transmitter as:

$$s_k(t) = \sum_{\tau_l^k \in \phi^k} \delta(t - \tau_l^k)$$

2.2.3 Fraction of molecules received by a passive receiver of non-negligible volume

Consider a receiver of radius a placed at the origin, and a transmitter at a location \vec{x} from the origin. In this section, we derive the fraction of molecules received by a receiver of non-negligible volume.

Note that the probability of a molecule being at a location \vec{r} at time t is given as:

$$c(\vec{r} - \vec{x}, t) = \frac{1}{(4\pi Dt)^{3/2}} \exp \left(\frac{-|\vec{r} - \vec{x}|^2}{4Dt} \right)$$

For a passive receiver of non-negligible volume, we need to integrate this expression over all points inside the receiver.

$$= \int_0^a \int_0^{2\pi} \int_0^\pi c(r - x, t) r^2 \sin\theta d\theta d\phi dr$$

Note that $|\vec{r} - \vec{x}|^2 = r^2 + x^2 - 2rx \cos\theta \sin\phi$. To solve the integral, we apply the following identities:

$$\begin{aligned}
 &\int_0^\pi \exp(b \cos w) dw = \pi I_0(b) \\
 &\int_0^\pi \sin(2\mu w) J_{2\nu}(2b \sin w) dw = \pi \sin(\mu\pi) J_{\nu-\mu}(b) J_{\mu+\nu}(b) \\
 &I_0(b) = J_0(jb) \\
 &J_{-1/2}(jb) J_{1/2}(jb) = \frac{1}{2\pi b} (\exp(2b) - \exp(-2b))
 \end{aligned}$$

$$\begin{aligned}
 &= \int_0^a \int_0^{2\pi} \int_0^\pi c(r-x, t) r^2 \sin\theta d\theta d\phi dr \\
 &= \int_0^a \int_0^{2\pi} \int_0^\pi \frac{1}{(4\pi Dt)^{3/2}} \exp\left(\frac{-r^2-x^2}{4Dt}\right) \exp\left(\frac{2rx \sin\theta \cos\phi}{4Dt}\right) r^2 \sin\theta d\theta d\phi dr \\
 &= \frac{1}{(4\pi Dt)^{3/2}} \int_0^a \int_0^\pi \exp\left(\frac{-r^2-x^2}{4Dt}\right) 2\pi I_0\left(\frac{2rx \sin\theta}{4Dt}\right) r^2 \sin\theta d\theta dr \\
 &= \frac{1}{(4\pi Dt)^{3/2}} \int_0^a \int_0^\pi \exp\left(\frac{-r^2-x^2}{4Dt}\right) 2\pi J_0\left(\frac{2jrx \sin\theta}{4Dt}\right) r^2 \sin\theta d\theta dr \\
 &= \frac{1}{(4\pi Dt)^{3/2}} \int_0^a \exp\left(\frac{-r^2-x^2}{4Dt}\right) 2\pi^2 J_{-1/2}\left(\frac{jrx}{4Dt}\right) J_{1/2}\left(\frac{jrx}{4Dt}\right) r^2 dr \\
 &= \frac{1}{(4\pi Dt)^{3/2}} \int_0^a \exp\left(\frac{-r^2-x^2}{4Dt}\right) 2\pi^2 \frac{4Dt}{2\pi rx} \left(\exp\left(\frac{2rx}{4Dt}\right) - \exp\left(-\frac{2rx}{4Dt}\right)\right) r^2 dr \\
 &= \frac{1}{x(4\pi Dt)^{1/2}} \int_0^a \left(\exp\left(\frac{-(r-x)^2}{4Dt}\right) - \exp\left(\frac{-(r+x)^2}{4Dt}\right)\right) r dr \\
 F(x, t) &= \frac{1}{2} \left[\operatorname{erf}\left(\frac{a-x}{\sqrt{4Dt}}\right) - \operatorname{erf}\left(\frac{a+x}{\sqrt{4Dt}}\right) \right] + \frac{1}{x} \sqrt{\frac{Dt}{\pi}} \left[\exp\left(-\frac{(R+x)^2}{4Dt}\right) - \exp\left(-\frac{(R-x)^2}{4Dt}\right) \right]
 \end{aligned}$$

2.2.4 Molecules received by a receiver in the system

Passive receivers do not interfere with each other, so the total number of molecules received by a receiver is simply the sum of the molecules reaching the receiver from each transmitter. Under the assumption that the diffusion of each molecule is independent, we can arrive at the expression through superposition.

So, the number of molecules received by the n^{th} receiver due to all emissions of all transmitters

$$N_n(t) = \sum_k \sum_l b_l^{kn}(t)$$

where $b_l^{kn}(t)$ is a Bernoulli RV with success probability $F(\|x_k - x_n\|, t - \tau_l^k)$.

The expected number of molecules received at time t can be computed as follows:

$$\begin{aligned}
 E[N_n(t)] &= E \left[\sum_k \sum_l b_l^{kn}(t) \right] \\
 &= E \left[\sum_{x_k \in \Pi_{T_x} | x_n \tau_l^k \in \phi_k} \sum E[b_l^{kn}(t)] \right] \\
 &= E \left[\sum_{x_k \in \Pi_{T_x} | x_n \tau_l^k \in \phi_k} \sum F(\|x_k - x_n\|, t - \tau_l^k) \right] \\
 &= \int_{\mathcal{R}^3} \lambda_{T_x} \sum_{\tau_l^k \in \phi_k} F(\|x - x_n\|, t - \tau_l^k) dx
 \end{aligned}$$

Appropriate decoding schemes can further be designed to infer the reception of information and corresponding error probabilities.

3 Multiple Transmitters and Fully Absorbing Receivers in 3D

In this section, we apply the techniques presented in [5] to the system model presented in the previous section.

3.1 System Model

The system is the same as the one considered in the previous section, except that the receivers are now fully absorbing. For clarity, we describe the system model below:

- Transmitters and receivers are randomly placed in 3D space. The transmitters are simply points. The receivers are spheres of radius a .
- The positions of the centers of the receivers are determined by a homogeneous Poisson point process.
- The emission of molecules from the transmitters is asynchronous. It is controlled by independent time PPs with the same intensity function that represent the propensity function of a chemical reaction.
- The medium is considered unbounded, where the molecules can diffuse with a constant diffusion coefficient D . The molecules do not undergo degradation.
- The receivers are fully absorbing i.e the molecules are removed from the system as soon as they hit a receiver for the first time.

3.2 System Analysis

3.2.1 Transmitter and Receiver Locations

The position of the n^{th} receiver x_n is a random variable belonging to a homogeneous Poisson Point Process $\Pi_{R_x} \in \mathcal{R}^3$ with intensity λ_{R_x} .

As derived earlier, the position of the k^{th} transmitter x_k is approximated by a random variable belonging to a homogeneous Poisson Point Process $\Pi_{T_x} \in \mathcal{R}^3$ with intensity λ_{T_x} .

3.2.2 Transmitted Signal

The emissions of the k^{th} transmitter are determined by a time Poisson Point Process ϕ with non-homogeneous intensity $\rho(t)$. The points belonging to the time PP represent the time instants at which the transmitter releases a molecule. Hence, we can write the signal transmitted by the k^{th} transmitter as:

$$s_k(t) = \sum_{\tau_l^k \in \phi^k} \delta(t - \tau_l^k)$$

3.2.3 Hitting rate for an individual receiver

Consider a single fully absorbing receiver of radius R at a distance r from a point transmitter. The hitting rate of molecules at a time t is given by the following expression:

$$f(r, t) = \frac{R}{r} \frac{r - R}{\sqrt{4\pi Dt^3}} \exp\left(-\frac{(r - R)^2}{4Dt}\right)$$

The number of molecules that are absorbed by the receiver within time t is given as:

$$N(t) = \int_0^t f(r, \tau) d\tau$$

3.2.4 Interference due to presence of multiple receivers

Unlike receivers, fully absorbing receivers interfere with each other. If some molecule is absorbed by a particular receiver, it cannot be absorbed by other receivers. The key idea in modelling this effect is to consider the other receivers as sources of negative molecules.

We first illustrate this model by considering one transmitter with two fully absorbing receivers. Consider a target receiver centered at a point C_R located at a distance r_R from the transmitter. The second receiver, the interferer, is centered at a point C_I located at a distance r_I from the transmitter. The distance between the centres of the two receivers is $d_{C_I C_R}$.

Let the transmitter transmit N molecules. We are interested in determining the absorption rates for both receivers, these are denoted as $n_R(t)$ and $n_I(t)$ respectively. For the interferer, we consider that it releases negative molecules according to its absorption profile, i.e the molecules that are absorbed in the interval $(t, t + dt)$ are released as negative molecules interfering with the other receiver in the system.

Note that for the receiver R , $Nf(r_R, t)$ is the absorption rate for the molecules emitted by the transmitter. For the interference term, we integrate over each interval $(\tau, \tau + d\tau)$ considering that it releases $n_I(\tau)$ molecules at that instant. Hence, the overall equation for the absorption rate of the receiver R is given as:

$$\begin{aligned} n_R(t) &= Nf(r_R, t) - \int_0^t n_I(\tau) f(d_{C_I C_R}, t - \tau) d\tau \\ n_R(t) &= Nf(r_R, t) - n_I(t) \star f(d_{C_I C_R}, t) \end{aligned}$$

Note that in this system, we arbitrarily assigned one of the receivers to be the target receiver while the other was the interferer. By symmetry arguments, we can also write the absorption rate for the interferer by interchanging the roles. Thus, we get the following system of equations:

$$\begin{aligned} n_R(t) &= Nf(r_R, t) - n_I(t) \star f(d_{C_I C_R}, t) \\ n_I(t) &= Nf(r_I, t) - n_R(t) \star f(d_{C_I C_R}, t) \end{aligned}$$

Solving this system of integral equations will yield the absorption rates for both the receivers. These expressions can then be integrated to calculate the number of molecules reaching each receiver within time t .

3.2.5 Molecules received by a receiver in the system

Extending the discussion above, for each receiver x_n all the other receivers x_i will act as interferers. Generalizing, we get the following system of equations for the absorption rates of all the receivers corresponding to a single transmitter x_k transmitting N molecules at $t = 0$:

$$n_n(t) = Nf(\|x_k - x_n\|, t) - \sum_{i \neq n} n_i(t) \star f(\|x_i - x_n\|, t) \quad \forall i, n \text{ s.t. } x_i \in \Pi_{R_x}$$

Considering that the transmitted signal for our system is a Dirac delta train, the contribution from the transmitter will be:

$$n_n(t) = \sum_{\tau_i^k \in \phi_k} f(\|x_k - x_n\|, t - \tau_i^k) - \sum_{i \neq n} n_i(t) \star f(\|x_i - x_n\|, t) \quad \forall i, n \text{ s.t. } x_i \in \Pi_{R_x}$$

Note that the interference term does not change since we are already considering the negative retransmission of all the molecules received by the receiver since $t = 0$. Similarly applying the superposition principle, we can write the overall absorption rate corresponding to the transmissions from all the transmitters in the system as follows:

$$n_n(t) = \sum_{x_k \in \Pi_{T_x}} \sum_{\tau_i^k \in \phi_k} f(\|x_k - x_n\|, t - \tau_i^k) - \sum_{i \neq n} n_i(t) \star f(\|x_i - x_n\|, t) \quad \forall i, n \text{ s.t. } x_i \in \Pi_{R_x}$$

Solving this complex system of equations numerically would yield the absorption rates for all receivers which can then be used to calculate the number of molecules reaching each receiver. Note that here, we have considered the interferer to be located at the center of the receiver. In [5], other approximations such as the surface interferer and the barycenter interferer have been analyzed. We leave the generalization of the above equations to these interferer models outside the scope of this term paper.

4 Multiple Transmitters and Receivers in a duct-like channel

In this section, we extend the system model presented in [8] to a system with multiple transmitters and receivers.

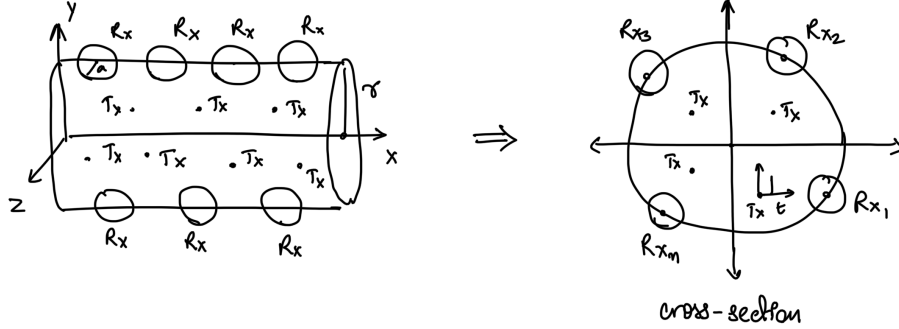


Figure 2: Multiple transmitters and receivers in a duct channel

4.1 System Model

The system model is described as follows:

- A straight infinite cylindrical duct of radius a is considered. This is the physical channel.
- The duct has a fluid of fixed viscosity that moves in steady laminar flow along the axis z , following a fixed radial velocity profile.
- The transmitters are simply points present inside the duct. The emission of molecules is governed by a time PP of intensity $\rho(t)$
- The receivers are embedded within the duct boundary. The receivers are sphere of radius R , with the centres lying on the duct boundary. The boundary is fully reflective in regions where the receivers are absent.
- The molecules can diffuse with a constant diffusion coefficient D . They are not degradable.

4.2 Analysis for Passive Receivers

4.2.1 Transmitter and Receiver Locations

The receiver centres lie on the walls of the duct. These points are governed by a homogeneous Poisson Point Process Π_{R_x} with intensity λ_{R_x} . Note that if the location of the n^{th} receiver x_n is written in cylindrical coordinates (r, ϕ, z) , r will be fixed at a , while z and ϕ will be random variables distributed over $[0, \infty)$ and $(-\pi, \pi]$ respectively.

The transmitter locations are governed by a homogeneous Poisson Point Process Π_{T_x} with intensity λ_{T_x} . Note that here we assume that all the passive receivers are transparent, i.e the transmitters can be placed within the receiver areas and particles can freely pass through as well. Note that if the location of the k^{th} transmitter x_k is written in cylindrical coordinates (r, ϕ, z) , r , z and ϕ will be random variables distributed over $[0, a)$, $[0, \infty)$ and $(-\pi, \pi]$ respectively.

We further posit that the transmitter locations remain fixed - unaffected by the flow of the fluid in the duct. This is a reasonable assumption since we are only looking at the relative motion of the particles and transmitters with respect to the fluid in the system.

4.2.2 Transmitted Signal

As considered in earlier sections, the signal transmitted by the k^{th} transmitter is:

$$s_k(t) = \sum_{\tau_i^k \in \theta^k} \delta(t - \tau_i^k)$$

where θ_k is the non-homogeneous time PP with intensity function $\rho(t)$

4.2.3 Solutions to the advection-diffusion equation

In the presence of a moving fluid in the channel, the probability of finding a molecule at a location r at time t is governed by the advection-diffusion equation:

$$\frac{\partial}{\partial t}p(r, t) = D\nabla^2p(r, t) - \nabla \cdot p(r, t)\vec{v}(r)$$

For a Newtonian fluid of viscosity η , the velocity profile is given as:

$$v(r) = 2v_{eff} \left(1 - \frac{r^2}{a^2}\right)$$

where $v_{eff} = |\partial_x P|a^2/8\eta$ is the mean velocity in the channel, $\partial_x P$ being the applied pressure gradient.

The Peclet number characterizes the relative importance of the competing advection and diffusion processes.

$$P_e = \frac{v_{eff}a}{D}$$

For the considered channel, with a single transmitter at the origin releasing a single molecule at $t = 0$, the advection-diffusion equation simplifies to the following:

$$\frac{\partial}{\partial t}p(r, t) = D\nabla^2p(r, t) - v(r)\frac{\partial}{\partial x}p(r, t)$$

The corresponding boundary condition is $\frac{\partial}{\partial r}p(r, t) = 0$, and the initial condition is given as $p(z, r, \phi, t = 0) = \delta(x)/\pi a^2$.

Once we have obtained the probability $p(z, r, \phi, t)$, we can obtain the observation probability for each receiver by integrating over the active volume of the receiver (note that since the centre is on the duct wall, only half of the receiver sphere lies inside the channel)

$$P_n(t) = \int_V *_{R_x} p(z, r, \phi, t) dV$$

We now consider two specific cases for which the advection-diffusion equation has an analytical solution - the dispersion regime and the flow-dominated regime.

Dispersion Regime:

The dispersion regime is characterized by the following condition:

$$\frac{d}{v_{eff}} \gg \frac{a^2}{4D}$$

which equivalently conveys that the time taken for particles to be moved by advection is much higher than the expected time for the particles to spread via diffusion.

In this regime, the solution to the advection-diffusion equation is given as:

$$p(z, r, \phi, t) = \frac{1}{\pi a^2} \frac{1}{\sqrt{4\pi D_{eff} t}} \exp\left(-\frac{(z - v_{eff}t)^2}{4D_{eff} t}\right)$$

where we note that the distribution is uniform across the cross-section. The effective diffusion coefficient is given by the Taylor-Aris equation:

$$D_{eff} = D \left(1 + \frac{1}{48} \left(\frac{v_{eff}a}{D}\right)^2\right)$$

Flow-dominated Regime:

The flow-dominated regime is characterized by the following condition:

$$\frac{d}{v_{eff}} \ll \frac{a^2}{4D}$$

Here advection happens much faster compared to diffusion.

In the flow-dominated regime, only the particles transmitted by the transmitters that lie in the receivers areas will be counted. Rest of the molecules flow away under the effect of advection.

4.2.4 Molecules received by a receiver in the system

As done in previous sections, the total number of molecules absorbed by each receiver can be calculated by applying superposition techniques.

5 Partially Counting Fully Absorbing Receivers

In this section, we analyse the system presented in [11].

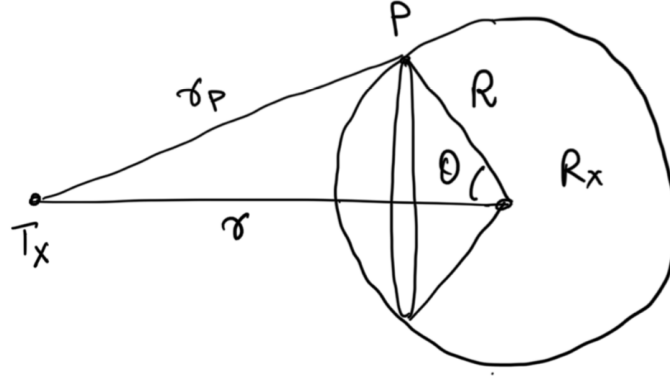


Figure 3: Partially Counting Fully Absorbing Receivers

5.1 System Model

The system model is visualized in Figure 3. It is described as follows:

- A spherical receiver R_x of radius R is placed at the origin.
- A point transmitter T_x is located at a point \vec{r}_0 .
- Only the angular region upto the angle θ is active - molecules that hit this region are considered to be received, while the rest are just absorbed.

5.2 System Analysis

5.2.1 Limiting angular distribution of molecules hitting the receiver

This section refers to [12] for the derivation.

Consider a particle transmitted by T_x placed at \vec{r}_0 . The concentration at any general point \vec{r} is obtained by solving the diffusion equation:

$$\frac{\partial}{\partial t} c(\vec{r}, t) = D \nabla^2 c(\vec{r}, t)$$

with the initial condition $c(\vec{r}, 0) = \delta(\vec{r} - \vec{r}_0)$ and the absorbing boundary condition $c(\vec{r}, t)|_{\vec{r} \in \Omega_{R_x}} = 0$ where Ω_{R_x} denotes the surface of the receiver. The outgoing flux at \vec{r} is then obtained as:

$$J(\vec{r}, t) = -D \frac{\partial}{\partial \hat{n}} c(\vec{r}', t)|_{\vec{r}' = \vec{r}}$$

from which we can calculate the eventual hitting probability:

$$P_H(\vec{r}) = \int_0^{\infty} J(\vec{r}, t) dt$$

Integrating the diffusion equation over time, we get:

$$\int_0^\infty \frac{\partial}{\partial t} c(\vec{r}, t) dt = \int_0^\infty \nabla^2 c(\vec{r}, t) dt$$

$$c(\vec{r}, \infty) - c(\vec{r}, 0) = D \nabla^2 C(\vec{r}, t)$$

where $C(\vec{r}, t) = \int_0^\infty c(\vec{r}, t) dt$. Applying the initial condition and assuming that the molecule is eventually absorbed, we get an equation for $C(\vec{r}, t)$

$$D \nabla^2 C(\vec{r}, t) = -\delta(\vec{r} - \vec{r}_0)$$

Comparing to the Poisson equation for electrostatic potential, we see that $C(\vec{r}, t)$ can be thought of as the potential due to a point charge placed at a location \vec{r}_0 . The magnitude of the corresponding point charge would be $q = \frac{1}{4\pi D}$

Correspondingly, the eventual hitting probability can be written as:

$$P_H(\vec{r}) = -D \int_0^\infty \frac{\partial}{\partial \hat{n}} c(\vec{r}, t) dt = -D \frac{\partial}{\partial \hat{n}} C(\vec{r}, t)$$

The absorbing boundary is analogous to a grounded conducting sphere that can absorb all charge. The eventual hitting probability corresponds to the electric field due to the equivalent charge.

Let us now look at the considered system. We are interested in finding the eventual hitting probability for point P , located at an angle θ as shown in Figure 3. Following the electrostatic analogue described above, we will first solve for the electrostatic potential by the method of images.

Let us assume the image charge q' is located at \vec{r}' . The electrostatic potential at \vec{r} is then:

$$\phi(\vec{r}) = \frac{q}{|\vec{r} - \vec{r}_0|} + \frac{q'}{|\vec{r} - \vec{r}'|}$$

The sphere is grounded, hence potential at the surface of the sphere must be zero. This gives:

$$\frac{q}{\sqrt{R^2 + r_0^2 - 2Rr_0 \cos(\theta)}} + \frac{q'}{\sqrt{R^2 + r'^2 - 2Rr' \cos(\theta)}} = 0$$

Solving this keeping in mind that the equation holds for all θ gives $r' = \frac{R^2}{r_0}$ and $q' = -\frac{qR}{r_0}$

Therefore for any point \vec{r} at an angle θ with respect to the origin the electrostatic potential is:

$$\phi(\vec{r}) = \frac{q}{\sqrt{r^2 + r_0^2 - 2rr_0 \cos(\theta)}} - \frac{qR/r_0}{\sqrt{r^2 + R^4/r_0^2 - 2rR^2 \cos(\theta)/r_0}}$$

From this, we can get the electric field as:

$$E(\vec{r}) = -\nabla \phi = \frac{q((r - r_0 \cos \theta)\hat{r} + r_0 \sin \theta \hat{\theta})}{[r^2 + r_0^2 - 2rr_0 \cos(\theta)]^{3/2}} - \frac{qR/r_0((r - R^2 \cos \theta/r_0)\hat{r} + R^2 \sin \theta/r_0 \hat{\theta})}{[r^2 + R^4/r_0^2 - 2rR^2 \cos(\theta)/r_0]^{3/2}}$$

Subsequently, the hitting probability at P is just the electric field at P multiplied by $-D$

$$P_H(\vec{r}_P) = \epsilon(\theta) = \frac{1}{4\pi R r_0} \frac{1 - R^2/r_0^2}{[1 - 2R \cos \theta/r_0 + R^2/r_0^2]^{3/2}}$$

Hence the marginal distribution for the angle θ as $t \rightarrow \infty$ is:

$$p_\infty(\theta) = 2\pi R^2 \sin \theta \frac{1}{4\pi R r_0} \frac{1 - R^2/r_0^2}{[1 - 2R \cos \theta/r_0 + R^2/r_0^2]^{3/2}}$$

5.2.2 Hitting probability for active region

Consider a small absorbing sphere of radius dr at the point P. The probability of absorption of molecules within time t can be obtained as:

$$p_P(t)^S = \frac{dr}{r_P} \operatorname{erfc} \left(\frac{r_P - dr}{\sqrt{4Dt}} \right) \sim \frac{dr}{r_P} \operatorname{erfc} \left(\frac{r_P}{\sqrt{4Dt}} \right)$$

However, this is not exactly the probability of absorption at P. This is because some part of the small sphere considered lies inside the receiver region, and hence it is not active. The region of the small sphere that is active is entirely dependent on the angle θ . This effect is modeled by multiplying an angle factor and a time factor. We write the overall hitting probability as:

$$p_P(t) = K p_P(t)^S T(\theta) \phi(t)$$

Here K represents the probability that the molecule is absorbed at this specific sphere at P and not any other spheres. If the probability of absorption for the entire sphere is $p(t)$, K can be written as:

$$K = 1 - (p(t) - p_P(t))$$

Thus

$$p_P(t) = (1 - (p(t) - p_P(t))) p_P(t)^S T(\theta) \phi(t) \sim (1 - p(t)) p_P(t)^S T(\theta) \phi(t)$$

Note that there are multiple spheres at the same angle θ . This number is simply given by the total circumference of the ring divided by the diameter of each small sphere:

$$N_\theta = \frac{2\pi R \sin\theta}{2dr}$$

Hence, the probability of absorption within time t by any small sphere at an angle θ is given as:

$$p(\theta, t) = \frac{2\pi R \sin\theta}{2dr} (1 - p(t)) p_P(t)^S T(\theta) \phi(t) = \pi R \sin\theta (1 - p(t)) \frac{\operatorname{erfc} \left(\frac{r_P}{\sqrt{4Dt}} \right)}{r_P}$$

Next, we derive the two factors by considering the limiting distributions.

As $t \rightarrow \infty$, $p(\theta, \infty) = p_\infty(t)$

$$\lim_{t \rightarrow \infty} p(\theta, t) = \pi R \sin\theta \left(1 - \frac{R}{r_0}\right) \frac{1}{r_P} T(\theta) \lim_{t \rightarrow \infty} \phi(t) = 2\pi R^2 \sin\theta \epsilon(\theta)$$

which gives:

$$T(\theta) = \frac{2Rr_P \epsilon(\theta)}{\left(1 - \frac{R}{r_P}\right) \lim_{t \rightarrow \infty} \phi(t)}$$

For deriving $\phi(t)$, we consider the fact that if the entire region of the receiver is active, the hitting probability should be the same as that of a fully absorbing receiver. That is, if we consider the total hitting probability:

$$F(\theta, t) = \int_0^\theta p(\alpha, t) d\alpha$$

Then

$$F(\pi, t) = p(t) = \frac{R}{r_0} \operatorname{erfc} \left(\frac{r_0 - R}{\sqrt{4Dt}} \right)$$

This gives:

$$\phi(t) = \frac{p(t)}{\pi R(1-p(t)) \int_0^\pi \frac{\sin\theta}{r_P} \operatorname{erfc}\left(\frac{r_P}{\sqrt{4Dt}}\right) T(\theta) d\theta}$$

Note that $r_P = \sqrt{r_0^2 + R^2 - 2Rr_0\cos\theta}$ is also a function of θ .

With this, we have entirely computed the hitting probability $p(\theta, t)$. If we consider the active region to be upto the angle α , the total hitting probability is $F(\alpha, t)$ as demonstrated above.

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