Chapter 2
Passive Molecular Communication
Through Absorbers

Abstract In this chapter, passive molecular communication (PMC) is introduced for the cases in which a receiver nanomachine (RN) is assumed to be an absorber to take messenger molecules inside. After the molecule emission process of a transmitter nanomachine (TN) is discussed, the diffusion of the emitted molecules is elaborated by giving the required details of random walk and diffusion equations. Then, the molecule reception process of RN (i.e., an absorber of messenger molecules) is detailed. By incorporating the mathematical models of the emission, diffusion, and reception processes, unified models are introduced for PMC. Finally, communication theories and techniques devised for PMC are introduced.

2.1 A Communication Architecture for PMC

The first step towards modeling the passive molecular communication (PMC) systems is to give an abstract communication architecture which can reflect the main functionalities of PMC as shown in Fig. 2.1. The PMC defined in this architecture can be divided into three main phases. The first phase is the emission of molecules. In this phase, the transmitter nanomachine (TN) emits the messenger molecules into the medium. The second phase includes the diffusion of molecules emitted by the TN. The last phase is the reception of molecules. In this phase, the receiver nanomachine (RN) receives molecules in its close proximity. Throughout this chapter, the RN is assumed to perfectly absorb the molecules that contact with its surface. In other words, the RN is assumed to be a perfect absorber and thus, the concept of the PMC with perfect absorber is introduced in this chapter. In the following sections, these three phases are elaborated in detail.
2.2 Emission of Molecule

In PMC, the TN is responsible for the emission of messenger molecules. The emitted messenger molecules carry information by propagating from the TN to the RN. In nature, there are many information-carrying messenger molecule types used for different vital tasks in the biological systems. Endocrine hormones, local mediators such as cytokines, neurotransmitters (e.g., dopamine, histamine), intracellular messengers (e.g., and cyclic AMP), and DNA/RNA molecules are the examples of the messenger molecules used in the biological systems. Furthermore, the messenger molecules can also be synthesized for specific purposes as demonstrated in drug delivery by, for example, using nanoparticles to target particular tissue types [30,35].

Let us assume that the TN is able to synthesize and emit a messenger molecule type in the medium with an emission rate, i.e., $\eta$. Let us also suppose that $\bar{S}$ denotes the molecule waiting to be emitted in TN and $\tilde{S}$ denotes the messenger molecule $\tilde{S}$ that has been emitted and started to diffuse in the medium as shown in Fig. 2.2. Hence, the molecule emission of TN can be characterized by a transition from $\bar{S}$ to $\tilde{S}$:

$$\text{Emission of } S : \bar{S} \xrightarrow{\eta} S$$  \hspace{1cm} (2.1)

Let us assume that $x_1(t)$ and $x_2(t)$ are the number of molecules $\bar{S}$ and $\tilde{S}$, respectively, and initially, $x_1(0) = n$ and $x_2(0) = 0$. Note that $x_2(t) = n - x_1(t)$ due to the fact that $x_1(t) + x_2(t) = n$. Based on the emission rate $\eta$, the time derivatives of $x_1(t)$ and $x_2(t)$ can be given as

$$\frac{dx(t)}{dt} = Ax(t)$$  \hspace{1cm} (2.2)
2.2 Emission of Molecule

where

\[ x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}, \quad A = \begin{bmatrix} -\eta & 0 \\ \eta & 0 \end{bmatrix} \] (2.3)

For the initial condition \( x_1(0) = n \), the solution of (2.2) can be given by

\[ x_1(t) = ne^{-\eta t}, \quad x_2(t) = n(1 - e^{-\eta t}) \] (2.4)

In fact, assuming that \( \bar{S} \) and \( S \) denote state 1 and state 2, respectively, the molecule emission process can be also viewed as a state transition from state 1 to state 2. In this case, a molecule \( \bar{S} \) may be either in state 1 or state 2. If it not emitted yet, it is in state 1. If it is emitted, it is no longer in state 1; it is in state 2.

Let \( p_i(t) \) be the probability that any selected particle is in state \( i \in \{1, 2\} \). Based on the emission rate \( \eta \), the time derivatives of \( p_i(t) \) can be derived by [19, 20, 26, 32]

\[ \frac{dp(t)}{dt} = Ap(t) \] (2.5)

where \( A \) has been already given in (2.3) and

\[ p(t) = \begin{bmatrix} p_1(t) \\ p_2(t) \end{bmatrix} \] (2.6)

Initially, there are only \( n \) molecules \( \bar{S} \). Hence, \( p_1(0) \) and \( p_2(0) \) can be given as \( p_1(0) = 1 \) and \( p_2(0) = 0 \). Based on this initial conditions, (2.5) can be solved to obtain \( p_1(t) \) and \( p_2(t) \) as

\[ p_1(t) = e^{-\eta t}, \quad p_2(t) = 1 - e^{-\eta t} \] (2.7)

Note that \( p_1(t) + p_2(t) = 1 \) due to the fact that any selected particle may be either \( \bar{S} \) (in state 1) or \( S \) (in state 2). Using \( p_i(t), i \in \{1, 2\} \), the joint probability distribution of \( x_1(t) \) and \( x_2(t) \), i.e., \( P(x_1, x_2, t) \), can be also given by the following multinomial distribution:

\[ P(x_1, x_2, t) = \frac{n! [p_1(t)]^{x_1} [p_2(t)]^{x_2}}{x_1! x_2!} \] (2.8)
Fig. 2.3 $P(x,t)$ is shown with time for the different $x$ values

Since the input signal consists of the emitted $S$ molecules, $x_2(t)$ is the input signal. Then, using $x_1(t) + x_2(t) = n$ and $p_1(t) + p_2(t) = 1$, $P(x_1,x_2,t)$ can be unconditioned in order to obtain the distribution of the input signal, i.e., $P(x_2,t)$, as follows:

$$P(x_2,t) = \frac{n![(1-p_2(t))^{n-x_2}][p_2(t)]^{x_2}}{(n-x_2)!x_2!} \tag{2.9}$$

By ignoring the subscript 2 in $x_2$ and substituting $p_2(t)$, the channel input distribution, i.e., $P(x,t)$, can be given by

$$P(x,t) = \frac{n![e^{-\eta t}]^{n-x}[1 - e^{-\eta t}]^x}{(n-x)!x!}$$

$$= \binom{n}{x} [e^{-\eta t}]^{n-x}[1 - e^{-\eta t}]^x \tag{2.10}$$

$P(x,t)$ characterizes the statistical dynamics of the molecule emission phase in the PMC. In order to visualize how $P(x,t)$ varies with the different values of $x$, in Fig. 2.3, by using $n = 100$ and $\eta = 0.02$, $P(x,t)$ is shown with time for the different values of $x$. As $x$ increases, the curve of $P(x,t)$ shifts right and becomes wider. This reveals that as $x$ increases, the variance of the time delay required to emit a specific number of molecules becomes higher. More specifically, as observed in Fig. 2.3, the delay required to emit 10 molecules ($x = 10$) changes from 2 s to 12 s while this is from 15 s to 40 s for the case of $x = 40$. In order to observe the effect of the emission rate $\eta$, in Fig. 2.4, $P(x,t)$ is plotted with time for the different values of $\eta$. As $\eta$ increases, the curve of $P(x,t)$ shifts left and becomes more narrow. This shows that the delay and its variance can be improved by increasing the emission rate $\eta$. 
In the following section, the diffusion phase of the emitted molecules is modeled by extensively discussing the physical background of the random walk and diffusion phenomena.

### 2.3 Diffusion of Molecules

After the messenger molecules are emitted into the medium by TN, they start to diffuse. Diffusion is the random movement of molecules due to the thermal energy. A molecule has a kinetic energy given as \( kT / 2 \) along each axis, where \( T \) is the absolute temperature and \( k \) is Boltzmann’s constant. Since each particle also has a mass \( m \) and a velocity \( v_x \) on the \( x \)-axis, the kinetic energy of the particle can be also expressed as \( mv_x^2 / 2 \). Such a kinetic energy inherently fluctuates. However, by equating \( \langle mv_x^2 / 2 \rangle \) with \( kT / 2 \), on the average,

\[
\langle v_x^2 \rangle = \frac{kT}{m}
\]  

(2.11)

can be written. Here, \( \langle \cdot \rangle \) denotes an average over time or over an ensemble of similar molecules. Using (2.11), the root-mean-square velocity can be also given by

\[
\langle v_x^2 \rangle^{1/2} = \left( \frac{kT}{m} \right)^{1/2}
\]  

(2.12)

The approximation of the root-mean-square velocity in (2.12) can be employed to estimate the instantaneous velocity of a molecule [10]. For example, the mass of a lysozyme molecule, which is a protein molecule, is \( m = 2.3 \times 10^{-20} \) g, and at the temperature 300 K (27°C), \( kT \) is \( 4.14 \times 10^{-14} \) gcm²/s². Hence, using (2.12), the
root-mean-square velocity can be estimated as $\langle v_x^2 \rangle^{1/2} = 1.3 \times 10^3 \text{ cm/s}$. Although the lysozyme molecule has such a considerable speed, in an aqueous medium, it frequently collides with the water molecules and thus, it cannot go far. This causes the protein molecule to execute a random walk by wandering around [10]. In order to understand the main principles of the diffusive spreading, the random walk throughout one dimension is first discussed. Then, this will be extended for two and three dimensions in the following section.

2.3.1 Random Walk

Let us consider one-dimensional random walk. Suppose that the molecules start at time $t = 0$ at position $x = 0$ and execute a random walk. The random walk of a molecule among these molecules is illustrated in Fig. 2.5. The random walk of the molecules is governed by the following rules:

1. Each molecule steps to the right or to the left once every $\tau$ seconds with the velocity $\pm v_x$ and the step length $\delta = \pm v_x \tau$.
2. The probabilities of going to the right or the left at each step are equal to each other and $1/2$. Note that the successive steps are statistically independent and the walk is not biased.
3. Each molecule moves independently of the other molecules. The molecules do not interact with each other.

Let us consider an ensemble of $N$ molecules and $x_i(n)$ be the position of the $i$th molecule after the $n$th step. Based on rule 1 defined above, the position of the $i$th molecule at time step $n$, i.e., $x_i(n)$, can be written as

$$x_i(n) = x_i(n-1) \pm \delta$$

(2.13)

Let us consider all of the $N$ molecules. Then, using rules 2 and 3, the + sign in (2.13) can be applied to the half of the molecules and the − sign can be applied to the other half. Hence, the mean displacement of the molecules after $n$th step, i.e., $\langle x(n) \rangle$, can be computed by
\[
\langle x(n) \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i(n)
\]
\[
= \frac{1}{N} \sum_{i=1}^{N} [x_i(n-1) \pm \delta]
\] (2.14)

Since the signs + and − are applied to the two half of the total number of particles, i.e., \( N \), the term \( \pm \delta \) in (2.14) can be approximated as 0 and \( \langle x(n) \rangle \) can be given by

\[
\langle x(n) \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i(n-1)
\]

\[
\langle x(n) \rangle = \langle x(n-1) \rangle
\] (2.15)

The physical interpretation of (2.15) reveals an interesting conclusion: the mean position of the molecules does not change from step to step. However, it is possible to determine how much the molecules spread. To this end, the average mean-square displacement \( \langle x(n) \rangle \) of the molecules, which is expressed as,

\[
\langle x^2(n) \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i^2(n)
\] (2.16)

can be used to measure the spreading. Using (2.13), \( x_i^2(n) \) can be given by

\[
x_i^2(n) = x_i^2(n-1) \pm 2\delta x_i(n-1) + \delta^2
\] (2.17)

By substituting \( x_i^2(n) \) in (2.16),

\[
\langle x^2(n) \rangle = \frac{1}{N} \sum_{i=1}^{N} [x_i^2(n-1) \pm 2\delta x_i(n-1) + \delta^2]
\]

\[
= \langle x^2(n-1) \rangle + \delta^2
\] (2.18)

can be written. Since all the molecules are assumed to be in origin at time 0, i.e., \( x_i(0) = 0 \ \forall i \), the mean-square displacement of the molecules at step 0 (or time 0), i.e., \( \langle x^2(0) \rangle \), is equal to 0. Thus, based on the result in (2.18), it can be easily inferred that \( \langle x^2(1) \rangle = \delta^2 \), \( \langle x^2(2) \rangle = 2\delta^2 \),..., \( \langle x^2(n) \rangle = n\delta^2 \). The physical interpretation of this result also reveals that the mean-square displacement increases with the step number \( n \) and the root-mean-square displacement increases with the square root of \( n \). Since each time step lasts for \( \tau \) second, the step number \( n \) can be easily expressed as \( n = t/\tau \) and using this result, the time-varying function of the mean-square displacement, i.e., \( \langle x^2(t) \rangle \), can be given as

\[
\langle x^2(t) \rangle = \left( \frac{t}{\tau} \right) \delta^2 = \left( \frac{\delta^2}{\tau} \right) t
\] (2.19)
By setting $\delta^2/2\tau$ as the diffusion coefficient of the molecules, i.e., $D = \delta^2/2\tau$ (cm$^2$/s), the mean-square displacement in (2.19) and the square root of this displacement can be also expressed as

$$\langle x^2 \rangle = 2Dt, \quad \langle x^2 \rangle^{1/2} = (2Dt)^{1/2}$$

(2.20)

Note that $t$ in $\langle x^2(t) \rangle$ is dropped for ease of illustration and thus, $\langle x^2 \rangle$ denotes $\langle x^2(t) \rangle$. The diffusion coefficient $D$ reflects how a type of molecules migrates at a given temperature. The diffusion coefficient mostly depends on the size of the particle, the structure of the medium and the absolute temperature. For example, the diffusion coefficient of a small molecule in water can be given as $D \simeq 10^{-5}$ cm$^2$/s. Such a particle diffuses a distance $x = 10^{-3}$ cm in $t \simeq x^2/2D = 5 \times 10^{-2}$ s. However, it requires $5 \times 10^4$ s to diffuse $x = 1$ cm.

Similar to the one-dimensional random walk of the molecule (along the $x$-axis), the two- and three-dimensional random walks can be analyzed by following the similar way given above. In fact, rule 1 and rule 3 can be directly applied to each axis, i.e., $x$, $y$, and $z$. Furthermore, the motion of the molecules in the $x$-, $y$-, and $z$-directions is statistically independent. Then, similar to $\langle x^2 \rangle = 2Dt$ as introduced in (2.20), $\langle y^2 \rangle = 2Dt$ and $\langle z^2 \rangle = 2Dt$. More specifically, in two dimensions, the square of the distance from the origin to the point $(x,y)$ is $r^2 = x^2 + y^2$. Thus, for two dimensions,

$$\langle r^2 \rangle = 4Dt,$$

(2.21)

and similarly, for three dimensions where $r^2 = x^2 + y^2 + z^2$

$$\langle r^2 \rangle = 6Dt,$$

(2.22)

can be given [10]. In Fig. 2.6, two-dimensional random walk simulation of a particle is shown for the step length $\delta = 0.01$ cm and the time step $\tau = 0.00001$ s. In the following section, the statistical characterization of the molecular random walk is presented based on the deterministic characterization introduced above.

### 2.3.2 Statistical Characterization of Random Walk

Here, the statistical characterization of one-dimensional random walk along the $x$-axis is first considered. Let us assume that a molecule steps to the right with a probability $p$ and to the left with a probability $q$. Since the movement of the molecule is one dimensional, $q = 1 - p^1$. Given that there are a total number of

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1Note that in the previous subsection, $p$ and $q$ have been set to $p = q = 1/2$. The analysis given here can be considered as a generalized version of the previous approach.
n steps, the probability that the molecule steps exactly \( k \) times to the right is given by the following binomial distribution:

\[
P(k; n, p) = \frac{n!}{k!(n-k)!} p^k q^{n-k}
\]  

(2.23)

The total displacement of the molecule at the end of \( n \) steps, i.e., \( x(n) \), can be found by extracting the number of left steps from the number of right steps as follows:

\[
x(n) = \left[ k - (n - k) \right] \delta = (2k - n) \delta
\]  

(2.24)

where \( \delta \) is the step length of the molecule as introduced in the previous subsection. Then, the mean displacement of the molecule, \( \langle x(n) \rangle \), can be written by

\[
\langle x(n) \rangle = (2k - n) \delta
\]  

(2.25)

Since \( k \) follows the binomial distribution in (2.23), \( \langle k \rangle \) in (2.25) can be given by \( \langle k \rangle = np \). Furthermore, the mean-square displacement of the molecule is

\[
\langle x^2(n) \rangle = \langle (2k - n) \delta \rangle^2 = 4 \langle k^2 \rangle - 4 \langle k \rangle (n + 2) \delta^2
\]  

(2.26)

where \( \langle k^2 \rangle = (np)^2 + npq \). Note that for the case of \( p = q = 1/2 \), \( \langle x(n) \rangle = 0 \) and \( \langle x^2(n) \rangle = n \delta^2 \) and this is an expected result as it has been already obtained in the previous subsection. The number of steps taken by each molecule is enormously high. For example, given the instantaneous velocity \( v_x = \delta / \tau \simeq 10^3 \text{ cm/s} \) and the diffusion coefficient \( D = \delta^2 / 2 \tau \simeq 10^{-6} \text{ cm}^2 / \text{s} \), the step rate of a molecule is
10\(^{12}\) steps/s. Therefore, the limiting behavior of the molecule displacement should be also considered. In fact, for the case of very large \(n\) and \(np\), one of the asymptotic limits of the binomial distribution in (2.23) is a Gaussian or normal distribution. Based on Stirling’s approximation of factorials, i.e.,

\[
n! \simeq (2\pi n)^{1/2}(n/e)^n,
\]

the Gaussian distribution which is equivalent to the binomial distribution in (2.23) can be given as

\[
P(k)dk = \frac{1}{\sqrt{2\pi \sigma^2}} e^{-\frac{(k-\mu)^2}{2\sigma^2}} dk
\]

where \(P(k)dk\) is the probability of finding the value of \(k\) between \(k+dk\), \(\mu = \langle k \rangle = np\), and \(\sigma^2 = npq\). By substituting \(x = (2k-n)\delta, dx = 2\delta dk, p = q = 1/2, t = n/\tau\) and \(D = \delta^2/2\tau\), (2.28) reduces

\[
P(x,t)dx = \frac{1}{\sqrt{4\pi Dt}} e^{\frac{-x^2}{4Dt}} dx
\]

where \(P(x,t)dx\) is the probability of finding a molecule between \(x\) and \(x+dx\). This is the probability density function of a standard normal distribution, i.e., \(\mathcal{N}(0, \sigma_x^2)\), with the variance \(\sigma_x^2 = 2Dt\) [10]. In Fig. 2.7, \(P(x,t)\) in (2.29) is plotted with varying \(x\) values and for the different values of \(t\). While its mean is always zero regardless of \(t\), the variance of \(P(x,t)\) increases with \(t\). Due to \(\sigma_x^2 = 2Dt\), the curve becomes wider as \(t\) increases. For the two- and three-dimensional random walk of the diffusion, such a normal distribution derived above for the \(x\)-axis can be directly applied to the \(y\)- and \(z\)-axis. In the following subsection, by taking into account the microscopic essentials of the random walk phenomenon, Fick’s equations (or called diffusion equations) are derived.
2.3 Diffusion of Molecules

Fig. 2.8 At time $t$, there are $N(x)$ and $N(x+\delta)$ molecules at position $x$ and $x+\delta$, respectively. At time $t+\tau$, half of $N(x)$ and $N(x+\delta)$ steps to the right while the other half of them steps to the left at time $t+\tau$.

2.3.3 Fick’s Equations

Fick’s equations characterize the spatial and temporal distributions of diffusing molecules. The derivation of Fick’s equations is possible to follow the basic principles of random walk. Let $N(x)$ and $N(x+\delta)$ be the number of particles at points $x$ and $x+\delta$ along the $x$-axis at time $t$, respectively, as shown in Fig. 2.8. In order to understand the spatial and temporal distributions of the molecules at points $x$ and $x+\delta$, there are two essential issues needed to be addressed [10]:

- How many particles will traverse unit area from the point $x$ to the point $x+\delta$ in unit time?
- What is the net flux in the $x$ direction, i.e., $J_x$?

At time $t+\tau$, half of the molecules at point $x$ steps across the dashed line from left to right and half of the molecules at point $x+\delta$ steps across the dashed line from right to left (see Fig. 2.8). Hence, the number of crossing to the right can be given as $-\frac{1}{2}[N(x+\delta)-N(x)]$. Dividing this expression by the unit area normal to the $x$-axis, i.e., $A$, and by the time interval $\tau$, the net flux $J_x$ can be found as

$$J_x = -\frac{1}{2} \frac{[N(x+\delta)-N(x)]}{A\tau} \quad (2.30)$$

As introduced previously, the diffusion coefficient $D$ can be given by $D = \frac{\delta^2}{2\tau}$. Then, by substituting $\tau = \frac{\delta^2}{2D}$, $J_x$ can be rewritten as

$$J_x = -D \frac{1}{\delta} \left[ \frac{N(x+\delta)}{A\delta} - \frac{N(x)}{A\delta} \right] \quad (2.31)$$

Since $A\delta$ is a unit volume, $\frac{N(x)}{A\delta}$ and $\frac{N(x+\delta)}{A\delta}$ in (2.31) are the concentrations of the molecules at points $x$ and $x+\delta$, respectively. Let $C(x)$ and $C(x+\delta)$ denote these concentrations, respectively. Then, (2.31) becomes

$$J_x = -D \frac{1}{\delta} [C(x+\delta) - C(x)] \quad (2.32)$$
The flux $J_x(x, t)$ enters from the left side of the box with the area $A$ and the flux $J_x(x + \delta, t)$ leaves from the right side of the box.

Finally, for $\delta \to 0$, the second term of $J_x$ becomes the derivative of $C(x)$ and this yields

$$J_x = -D \frac{\partial C}{\partial x} \quad (2.33)$$

Equation (2.33) is called as Fick’s first equation and it can be interpreted as follows. If the molecules are uniformly distributed, $\partial C/\partial x = 0$ and $J_x = 0$. In this case, the distribution does not change with time and the system is at equilibrium. If the concentration $C$ is a linear function of $x$, $\partial C/\partial x$ and $J_x$ are constant [10]. Based on the conservation of total number of the molecules, Fick’s second equation can be also derived by following the first equation in (2.33). Let us consider the box with the area of $A$ as shown in Fig. 2.9. During the time period $\tau$, the number of molecules entering from the left of the box is $J_x(x)A\tau$ while the number of molecules leaving from the right is $J_x(x + \delta)A\tau$. Since the molecules are neither created nor destroyed, the difference of the entering and leaving molecule concentration in the volume of the box, i.e., $A\delta$, must satisfy

$$[C(t + \tau) - C(t)] = - \frac{[J_x(x + \delta) - J_x(x)]A\tau}{A\delta} \quad (2.34)$$

Multiplying (2.34) by $1/\tau$, it can be expressed as

$$\frac{1}{\tau} [C(t + \tau) - C(t)] = - \frac{1}{\tau} \frac{[J_x(x + \delta) - J_x(x)]A\tau}{A\delta} = - \frac{1}{\delta} [J_x(x + \delta) - J_x(x)] \cdot \quad (2.35)$$
As $\tau \to 0$ and $\delta \to 0$, (2.35) becomes

$$\frac{\partial C}{\partial t} = -\frac{\partial J_x}{\partial x} \quad (2.36)$$

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (2.37)$$

Note that (2.37) is obtained by substituting (2.33) into (2.36). The final expression in (2.37) is known as Fick’s second equation or diffusion equation. In three dimensions, there should be two more terms for the $y$- and $z$-axis. Since the movement of molecules along different axes is independent, the flux along $y$- and $z$-axis can be directly written as $J_y = -D \partial C/\partial y$ and $J_z = -D \partial C/\partial z$, respectively. Furthermore, the vector of the fluxes, i.e., $\mathbf{J}$, is

$$\mathbf{J} = -D \nabla C \quad (2.38)$$

The one-dimensional Fick’s second equation in (2.37) can also be extended to the three dimension as

$$\frac{\partial C}{\partial t} = D \nabla^2 C \quad (2.39)$$

where $\nabla^2$ is the three-dimensional Laplacian, i.e., $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$. If the problem is assumed to be spherically symmetric, the flux, $J_r$, and Fick’s equation can be expressed by [10]

$$J_r = -D \frac{\partial C}{\partial r} \quad (2.40)$$

$$\frac{\partial C}{\partial t} = D \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial C}{\partial r} \right) \quad (2.41)$$

Up to now, it has been assumed that molecules freely diffuse in the medium. However, it is highly likely that molecules are exposed to an external force causing a drift velocity. For such cases, diffusion equations derived above require some modifications. To this end, let us consider that a molecule is subject to an externally applied force $F_x$ during its one-dimensional random walk along $x$-axis as depicted in Fig. 2.10. The force results in the acceleration of the particle towards the right side.
i.e., $a = F_x / m$, where $m$ is the mass of the molecule. The molecule always continues its one-dimensional random walk while the external force is applied to it. Due to the random walk, the molecule steps to the right or the left once every $\tau$ seconds with the velocity $+v_x$ and $-v_x$, respectively. In addition to these velocities, the molecule also has another average drag velocity term, i.e., $v_d$, which can be given as

$$v_d = \frac{a \tau}{2} = \frac{F_x \tau}{2m} \tag{2.42}$$

Hence, in each $\tau$, the molecule steps to the right with a distance $\delta_+ = v_x \tau + v_d \tau$ or it steps to the right with a distance $\delta_- = -v_x \tau + v_d \tau$ (see Fig. 2.10). These steps determine the physical characterization of the random walk with drift [10]. Based on these steps, Fick’s first and second equations in (2.33) and (2.37) can be modified as [10]

$$J_x = -D \frac{\partial C}{\partial x} + v_d C, \tag{2.43}$$

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v_d \frac{\partial C}{\partial x}. \tag{2.44}$$

For the details of the diffusion with drift, see [10]. Next, some of the solution approaches to diffusion equations are exemplified.

### 2.3.4 Example Solutions for Diffusion Equation

The solutions of diffusion equations can be obtained for different initial and boundary conditions. As these conditions vary, many different solutions can be obtained. In general, the solutions are either in the form of a series of error functions or in the form of a trigonometric series. The trigonometric series can be replaced by a series of Bessel functions for the case in which the diffusion takes place in a cylinder [17]. In the literature, there are many textbooks and research papers dealing with the solution of Fick’s equations (or diffusion equations). For example, [17] is an important textbook discussing the solution approaches to Fick’s equations extensively. Furthermore, the heat equation has the same form with Fick’s equations. Therefore, the textbooks on the heat equation can be also used to understand how diffusion equations are solved. For example, [14] is a prominent book which provides many important solutions of diffusion equations with respect to many different initial and boundary conditions. Some of the examples solutions can be given as follows.

Let us consider the one-dimensional diffusion equation in (2.37):

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \tag{2.45}$$
2.3 Diffusion of Molecules

It is easy to prove that

\[ C = \frac{K}{\sqrt{t}} e^{-\frac{x^2}{4Dt}} \]  

(2.46)
is a solution of (2.45) for an arbitrary constant \( K \) [17]. Let us assume that \( M \) molecules are instantaneously released at the origin of a cartesian coordinate system at \( t = 0 \). Then, using (2.46), \( M \) can be expressed as

\[
M = \int_{-\infty}^{\infty} C \, dx \\
= \int_{-\infty}^{\infty} \frac{K}{\sqrt{t}} e^{-\frac{x^2}{4Dt}} \, dx
\]

(2.47)

By changing the variable \( x \) as

\[
\frac{x^2}{4Dt} = a^2, \quad dx = 2\sqrt{Dt} \, da
\]

(2.48)

\( M \) can be written as

\[
M = 2K\sqrt{D} \int_{-\infty}^{\infty} e^{-a^2} \, da \\
= 2K\sqrt{\pi D}
\]

(2.49)

Hence, \( K = \frac{M}{2\sqrt{\pi D}} \) and by substituting \( K \) into (2.46), \( C \) can be given by

\[
C = \frac{M}{\sqrt{4\pi Dt}} e^{\frac{x^2}{4Dt}}
\]

(2.50)

Similarly, the two- and three-dimensional diffusion equations are, respectively, satisfied by

\[
C = \frac{K}{t} e^{-\frac{(x^2+y^2)}{4Dt}}, \quad C = \frac{K}{t^{3/2}} e^{-\frac{(x^2+y^2+z^2)}{4Dt}}.
\]

(2.51)

By following the similar steps used for the solution of one-dimensional diffusion equation, the solutions for two- and three-dimensional diffusion equations can be given as [17]

\[
C = \frac{M}{4\pi Dt} e^{-\frac{(x^2+y^2)}{4Dt}}
\]

(2.52)

\[
C = \frac{M}{(4\pi Dt)^{3/2}} e^{-\frac{(x^2+y^2+z^2)}{4Dt}}
\]

(2.53)
$C/M$ in (2.53) is plotted in Fig. 2.11. As $t$ increases, the curve becomes wider and its peak value (at $r = 0$) decreases. This is because molecules continuously diffuse and scatter in the medium as time proceeds.

Instead of the instantaneous emission, if the molecules are assumed to be emitted with an emission rate $\eta(t)$, then the concentration at a point distance $r = x^2 + y^2 + z^2$ at time $t$ is obtained by integrating (2.53) as follows [13]:

$$C = \int_0^t \frac{\eta(t')}{[4\pi D(t-t')]^{3/2}} e^{\frac{-r^2}{4D(t-t')}} dt'$$

(2.54)

If the emission rate $\eta(t)$ is constant, i.e., $\eta(t) = \eta$, then

$$C = \frac{\eta}{4\pi Dr} \text{erfc} \left( \frac{r}{\sqrt{4Dt}} \right)$$

(2.55)

where $\text{erfc}(-\cdot)$ is the complementary error function. Note that the details of this derivation can be found in [13]. In Fig. 2.12, (2.55) is plotted to show how $C$ varies with time. For the different values of $r$, it is observed that $C$ decreases with $r$. This is a clear result of the free diffusion of the molecules in an infinite medium. $C$ starts to converge as time proceeds. This stems from the characteristics of the complementary error function in (2.55).

Here, it is worth to note that for $M = 1$, the solution in (2.50) is equal to the probability density function of molecule position which has been already given in (2.29) as

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{\frac{-x^2}{4Dt}}$$

(2.56)
This means that the diffusion equation is satisfied by the probability density function of molecule position in one dimension. Using this distribution, the probability distribution of the delay required by a molecule to travel the distance $d$ can be derived as

$$f(t) = \frac{d}{\sqrt{4\pi Dt^3}} e^{-\frac{d^2}{4Dt}} \quad (2.57)$$

Furthermore, if there is a drift velocity $v$ in the medium, (2.56) and (2.57) become

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-vt)^2}{4Dt}} \quad (2.58)$$
$$f(t) = \frac{d}{\sqrt{4\pi Dt^3}} e^{-\frac{(vt-d)^2}{4Dt}} \quad (2.59)$$

In addition to the solutions given for the instantaneous and the constant emission patterns in (2.50), (2.52), (2.53), and (2.55), the solution of the diffusion equation can be also given for more generalized emission patterns of TN [2]. Here, some example solutions are given for diffusion equation with such generalized emission patters. Let first rewrite the diffusion equation in (2.39) as

$$\frac{\partial C}{\partial t} = D \nabla^2 C. \quad (2.60)$$

Let us assume a spherical coordinate system $(r, \theta, \phi)$, where $r$ denotes the distance to the origin and $\theta$ and $\phi$ are the zenith and azimuth, respectively. The non-dimensional variables $x$ and $\tau$ can be defined as

$$x = \frac{r}{a}, \quad \tau = \frac{Dt}{a^2} \quad (2.61)$$

---

2For the details of the derivations of (2.57)–(2.59), see [27, 28, 39].
where \( a \) is the radius of TN. Based on these variables, the modification of (2.60) yields

\[
\frac{\partial C}{\partial \tau} = \nabla^2 C \quad \text{for} \quad x > 1 \tag{2.62}
\]

where

\[
\nabla^2 \equiv \frac{1}{x^2} \left[ \frac{\partial}{\partial x} \left( x^2 \frac{\partial}{\partial x} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \tag{2.63}
\]

The secretion rate of molecules from the surface of TN and the concentration at infinite distance from the TN impose two boundary conditions:

\[
\frac{\partial C}{\partial x} = -\frac{aF_0(\theta, \phi)}{D} g(\tau) \quad \text{for} \quad x = 1 \tag{2.64}
\]

\[
C \to 0 \quad \text{as} \quad x \to \infty \tag{2.65}
\]

where \( g(\tau) \) and \( F_0(\theta, \phi) \) identify the time and spatial variation of the secretion from the surface of TN and they are assumed to be separable functions. Note also that \( x = 1 \) means \( r = a \) [see (2.61)]. The general method for the solution of (2.62) can be found in [2]. Here, the solutions are only introduced for the following four different cases:

- In the first case, the emission rate is assumed to be uniformly distributed on the spherical surface of TN and the time-dependence of the secretion is steady. Hence, for this case, the boundary condition in (2.64) can be identified as

\[
\frac{aF_0(\theta, \phi)}{D} = \hat{F}_0, \quad g(\tau) = H(\tau) \tag{2.66}
\]

where \( H(\tau) \) is a Heaviside step function and \( \hat{F}_0 \) is the normalized concentration which is independent of the direction. Based on this setting, the solution of (2.62) is

\[
C(\xi, \tau) = \frac{1}{1 + \xi} \left[ \text{erfc} \left( \frac{\xi}{2\sqrt{\tau}} \right) - e^{\xi + \tau} \text{erfc} \left( \frac{\xi + \tau}{2\sqrt{\tau}} \right) \right] \tag{2.67}
\]

where \( \xi = x - 1 \) is set for the simplification and \( \text{erfc}(\cdot) \) is the complementary error function. In Fig. 2.13, the time evolution of \( C(\xi, \tau) \) is shown for the different values of \( \xi \).

- If a simple directional preference is considered in the emission, then the boundary condition in (2.66) becomes

\[
\frac{aF_0(\theta, \phi)}{D} = \hat{F}_0 \cos \theta, \quad g(\tau) = H(\tau). \tag{2.68}
\]
Such a directional releasing pattern means that
- For $\theta = 0$, the TN releases molecules at a constant rate $D\hat{F}_0/a$ on its north pole. This is due to $\cos 0 = 1$.
- For $\theta = \pi$, the TN behaves like the RN and it absorbs molecules at the constant rate $D\hat{F}_0/a$ on its south pole due to $\cos \pi = -1$. Note that for the absorption, a constant external concentration of molecules is assumed to exist around the TN.
- The total secretion rate from the TN is zero since the TN emits and absorbs the same amount of molecules as $\theta$ changes from 0 to $2\pi$.

Based on this boundary condition, the solution is

$$C(\xi, \theta, \tau) = \frac{\cos \theta}{4(1 + \xi)^2} \left[ 2\text{erfc} \left( \frac{\xi}{2\sqrt{\tau}} \right) + 
+i \left( (2\xi + 1 + i)\text{erfc} \left( \sqrt{2i\tau} + \frac{\xi}{2\sqrt{\tau}} \right) e^{\xi+i(\xi+2\tau)} - 
- (2\xi + 1 - i)\text{erfc} \left( \sqrt{-2i\tau} + \frac{\xi}{2\sqrt{\tau}} \right) e^{\xi-i(\xi+2\tau)} \right] \right)$$

(2.69)

Although the given solution includes the complex terms, it always generates real values. The simplification of (2.69) also yields [2]

$$C(\xi, \theta, \tau) = \frac{\cos \theta}{2(1 + \xi)^2} \left[ \text{erfc} \left( \frac{\xi}{2\sqrt{\tau}} \right) + 
+ \text{Im} \left[ (2\xi + 1 - i)\text{erfc} \left( \sqrt{-2i\tau} + \frac{\xi}{2\sqrt{\tau}} \right) e^{\xi-i(\xi+2\tau)} \right] \right]$$

(2.70)
• If the emission of TN is assumed to be uniformly distributed on the surface of TN and exponentially decaying in time, the boundary condition becomes

\[
\frac{aF_0(\theta, \phi)}{D} = \hat{F}_0, \quad g(\tau) = H(\tau)e^{-p\tau}.
\]  

(2.71)

where \( p \) is a non-dimensional constant. Then, the corresponding solution is

\[
C(\xi, \tau) = \frac{1}{(1+\xi)(1+p)} \left[ -\text{erfc}\left(\frac{\xi}{2\sqrt{\tau}} + \sqrt{\tau}\right)e^{\xi+\tau} + 
\right.
\]

\[
+ \text{Re}\left[(1+i\sqrt{p})\text{erfc}\left(i\sqrt{p}\tau + \frac{\xi}{2\sqrt{\tau}}\right)e^{-p\tau+i\sqrt{p}\xi}\right]
\]

(2.72)

• If a preferred direction and an exponential decaying are assumed, then the boundary condition is

\[
\frac{aF_0(\theta, \phi)}{D} = \hat{F}_0 \cos \theta, \quad g(\tau) = H(\tau)e^{-p\tau}.
\]  

(2.73)

The corresponding solution can be given by

\[
C(\xi, \theta, \tau) = \frac{\cos \theta}{(1+\xi)^2(4+p^2)} \times 
\]

\[
\left[ \text{Re}\left[ -(p-2i)(2\xi + 1 + i)\text{erfc}\left(\sqrt{2i\tau + \frac{\xi}{2\sqrt{\tau}}}\right)e^{\xi+2\tau}\right] + 
\right.
\]

\[
+ \left[1-i\sqrt{p}(1+\xi)\right]\left[1+(1+i\sqrt{p})^2\right]\text{erfc}\left(i\sqrt{p}\tau + \frac{\xi}{2\sqrt{\tau}}\right)e^{-p\tau+i\sqrt{p}\xi}\right]
\]

(2.74)

Due to linearity, the superpositions of the solutions given above can be used to obtain solutions for many different boundary conditions. For example, for the boundary condition \( aF_0(\theta, \phi)/D = \hat{F}_0(1 + \cos \theta) \), the solution can be obtained by superposition of the solutions given in (2.67) and (2.69). Note that in order to determine the longtime and/or long-distance characteristics of the above given solutions, their limiting approximations should be evaluated. Such asymptotic evaluations can be found in [2]. With this subsection, Sect. 2.3 (diffusion of molecules) is ended. As depicted in Fig. 2.1, after the diffusion phase, in the phase of reception, the emitted molecules that are able to reach the close proximity of RN are received by the RN. In the following section, the reception of molecules is discussed.
2.4 Reception of Molecules

After the messenger molecules are emitted by the TN, they diffuse in the medium by following the physical rules introduced in the previous section. The molecules that are able to reach the close proximity of RN are received by the RN. Hence, RN can be viewed as an absorber such that it may either perfectly absorb the molecules contacting with its surface or use some specific surface receptors to receive the molecules. Throughout this chapter, the RN is assumed to perfectly absorb molecules (it is assumed to be a perfect absorber). Next, rate expressions are derived for the reception of molecules with a perfect absorber.

2.4.1 Reception Rate of Molecules with a Perfect Absorber

In PMC, the TN behaves like a source to emit molecules and the RN behaves like an absorber to receive molecules. The distribution of the molecules in the medium is not uniform. However, the distribution of molecule concentration reaches a steady state such that the concentration is higher near the TN and lower near the RN. In this limit, the diffusion equation in (2.39) reduces to

$$\nabla^2 C = 0 \tag{2.75}$$

For problems having spherical symmetry, (2.75) becomes

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dC}{dr} \right) = 0 \tag{2.76}$$

Let us assume that the RN is a spherical perfect absorber with radius $a$ in an infinite medium and directly receives any molecule reaching its surface (see Fig. 2.14). Therefore, the concentration at $r = a$ is 0. Furthermore, the concentration at $r = \infty$ is assumed to be $C_0$. Based on these boundary conditions, the solution of (2.76) is

$$C(r) = C_0 \left( 1 - \frac{a}{r} \right) \tag{2.77}$$

Fig. 2.14 The RN receives the messenger molecules which freely wander in close proximity of it. The RN can be viewed as an absorber to absorb the messenger molecules.
By using (2.40), the flux can be given by

$$J_r(r) = -DC_0 \frac{a}{r^2}$$  \hspace{1cm} (2.78)

The diffusive current rate $I_0$ at which molecules are absorbed by RN can be found by multiplying the flux $-J_r(a)$ by the surface area of RN (i.e., $4\pi a^2$) as follows:

$$I_0 = 4\pi DaC_0$$  \hspace{1cm} (2.79)

$I_0$ is the absorption rate of RN in molecules per second [10]. In fact, using the electrical analogy\(^3\) of the diffusive current problem, a general expression for the steady-state diffusive current (i.e., $I$) to a totally absorbing body of any shape and size can be given by [11]

$$I = 4\pi D\zeta C_0$$  \hspace{1cm} (2.80)

where $\zeta$ is the electrical capacitance of an isolated conductor in centimeter-gram-second (cgs) units. Using $I$ in (2.80), $I_0$ in (2.79) can be again derived as follows. The capacitance of spherical RN with radius $a$ is equal to $a$ in cgs (i.e., $\zeta = a$ for the spherical RN). By substituting $\zeta = a$ into (2.80), $I_0$ can be obtained as $I_0 = 4\pi DaC_0$.

Let us also assume that rather than the perfect absorber assumption, there are $N$ receptor batches on the surface of RN to absorb molecules. In order to find the absorption rate of such an RN, the electrostatic analogy and the general diffusive current expression $I$ in (2.80) can be used. In the electrostatic analogy, the spherical RN with $N$ receptor patches is analogous to the same size insulating sphere whose surface includes $N$ evenly distributed conducting disks (with radius $s$). The capacitance $\zeta$ of this sphere is [11]

$$\zeta = \frac{Ns a}{Ns + \pi a}$$  \hspace{1cm} (2.81)

The rate $I_1$ of the diffusion current to such a sphere can be found by substituting the capacitance $\zeta$ in (2.81) into the general diffusive current expression in (2.80) as follows:

$$I_1 = 4\pi D\zeta C_0$$

$$= 4\pi DC_0 \left( \frac{Ns a}{Ns + \pi a} \right)$$

$$= I_0 \left( \frac{Ns}{Ns + \pi a} \right)$$  \hspace{1cm} (2.82)

\(^3\)The electrical analogy of the diffusion current is based on the analogy between the time-independent diffusion equation $\nabla^2 C = 0$ and Laplace’s equation for the electrostatic potential $\phi$ in charge-free space, i.e., $\nabla^2 \phi = 0$. For the details, see [11].
2.4 Reception of Molecules

Note that as observed in (2.82), if the RN has receptors patches on its surface to absorb molecules, the diffusive current to the RN is just a scaled version of the current derived for the case in which the RN is a spherical perfect absorber. Similarly, using (2.80), the diffusion current to a one-side disklike absorber with radius $s$ can be obtained. The capacitance, $\zeta$, of this absorber is $\zeta = s/\pi$. Hence, by substituting this capacitance into (2.80), the diffusion current to this disklike absorber, i.e., $I_2$, can be given by

$$I_2 = 4DsC_0$$ (2.83)

The diffusion current expressions derived above are extensively used throughout the following sections. In addition to the particle absorption rate of RN, it is also possible to derive the probability that a molecule released by the TN is captured by the RN as introduced in the following section.

2.4.2 Capture Probability of Molecules with a Perfect Absorber

Suppose that a molecule is released by a spherical shell source with radius $b$ between the RN and another spherical shell absorber with radius $c$ as depicted in Fig. 2.15. The concentration is 0 at $r = a$ since the RN can perfectly absorb the incoming molecules. The concentration reaches to its maximum, i.e., $C_m$, at the source location ($r = b$) and then reduces again to 0 at $r = c$ since an absorber is assumed to be located at this location. Based on these boundary conditions, (2.76) has the following solution [10]:

$$C(r) = \begin{cases} 
\frac{C_m}{1 - \frac{a}{b}} \left(1 - \frac{a}{r}\right) & a \leq r \leq b \\
\frac{C_m}{1 - \frac{c}{b}} \left(1 - \frac{c}{r}\right) & b \leq r \leq c 
\end{cases}$$ (2.84)

The corresponding flux, i.e., $J_r(r)$, is

$$J_r(r) = \begin{cases} 
-DC_m \frac{a}{\left(1 - \frac{a}{b}\right) r^2} & a \leq r \leq b \\
DC_m \frac{c}{\left(\frac{c}{b} - 1\right) r^2} & b \leq r \leq c 
\end{cases}$$ (2.85)

Hence, the absorption rate of RN, i.e., $I_{in}$, can be derived by multiplying $J_r(a)$ with the surface area of RN ($4\pi a^2$) as follows

$$I_{in} = \frac{4\pi DC_m a}{1 - \frac{a}{b}}$$ (2.86)

Similarly, the absorption rate of the outermost shell with radius $c$, i.e., $I_{out}$, can be derived by multiplying $J_r(c)$ with the surface area of RN ($4\pi c^2$) as follows:

$$I_{out} = \frac{4\pi DC_m c}{\frac{c}{b} - 1}$$ (2.87)
Fig. 2.15 The RN absorbs the messenger molecules emitted by a spherical shell source with radius \( b \) which is between the RN and another spherical shell absorber with radius \( c \).

The ratio

\[
\frac{I_{\text{in}}}{I_{\text{in}} + I_{\text{out}}} = \frac{a(c - b)}{b(c - a)}
\]

(2.88)

can be viewed as the probability that a particle released at \( r = b \) will be absorbed by the RN at \( r = a \). For \( c \to \infty \), this probability reduces to

\[
\frac{I_{\text{in}}}{I_{\text{in}} + I_{\text{out}}} = \frac{a}{b}
\]

(2.89)

This ratio can be interpreted as the capture probability of RN in an infinite medium. Note that the capture probability can be also derived using the electrostatic analogy. For the details of this derivation, see [11]. Next, based on the principles of random walk, an expression is derived for mean time in which a molecule is captured by the RN after it is emitted by the TN. Hence, this time is called as mean time to capture [10].
2.4 Reception of Molecules

2.4.3 Mean Time to Capture

Let us assume that in a one-dimensional medium, a molecule is emitted at position $x = m$ by the TN and there are two RNs to capture the molecule at positions $x = 0$ and $x = b$. Let $W(m)$ be the mean time in which the molecule is captured by one of the RNs at $x = 0$ and $x = b$. Suppose that a molecule is released at a position $m$ (i.e., any position $m$) at time $t = 0$. It steps to the right or to the left a distance $\delta$ every $\tau$ seconds. At time $\tau$, the molecule will be at position $x + \delta$ with probability 1/2 or at position $x - \delta$ with probability 1/2. The mean times to capture from these positions are $W(x + \delta)$ and $W(x - \delta)$, respectively. Hence, the expected value of $W(x)$ is

$$W(x) = \tau + \frac{1}{2} [W(x + \delta) + W(x - \delta)] \tag{2.90}$$

By subtracting $W(x)$ from both sides and multiplying by $2/\delta$, (2.90) can be rearranged as

$$\frac{1}{\delta} [W(x + \delta) - W(x)] - \frac{1}{\delta} [W(x) - W(x - \delta)] + \frac{2\tau}{\delta} = 0 \tag{2.91}$$

For $\delta \to 0$, the first and second terms of (2.91) become the derivative of $W(x)$ and this yields

$$\frac{dW}{dx} \bigg|_{x} - \frac{dW}{dx} \bigg|_{x-\delta} + \frac{2\tau}{\delta} = 0 \tag{2.92}$$

Dividing both sides by $\delta$ and considering the definition of a derivative, (2.92) can be expressed as

$$\frac{d^2W}{dx^2} + \frac{1}{D} = 0 \tag{2.93}$$

where $D = \delta^2/2\tau$ as defined previously. Equation (2.93) can be solved for appropriate boundary conditions. At a position at which an adsorbing boundary conditions (it can be considered as RN) is located, the mean time to capture is 0, i.e., $W = 0$. Hence, for the case in which two absorbing RNs are located at $x = 0$ and $x = b$, $W(0)$ and $W(b)$ are both equal to 0. Then, for these boundary conditions, (2.93) has the solution [10]

$$W(x) = \frac{1}{2D} (bx - x^2) \tag{2.94}$$

For example, if a molecule is assumed to be released at $x = b/2$, then the mean time to capture, i.e., $W(b/2)$, is equal to $b^2/8D$. Furthermore, if the molecule is assumed
to be released anywhere in between \( x = 0 \) and \( x = b \) (uniformly between \( x = 0 \) and \( x = b \)), the mean time to capture, i.e., \( \tau \), can be found by averaging \( W(x) \) as follows:

\[
\tau = \frac{1}{b} \int_{0}^{b} W(x) dx = \frac{b^2}{12D} \tag{2.95}
\]

Two- or three-dimensional extension of (2.93) can be also given as

\[
\nabla^2 W + \frac{1}{D} = 0 \tag{2.96}
\]

where \( \nabla^2 \) is the two- or three-dimensional Laplacian. For example, let consider a circular absorber of radius \( s \) centered within an impermeable boundary of radius \( b \). By employing the electrical analogue as introduced in [1, 11], for the given setting, \( W(x) \) is

\[
W(x) = \frac{2b^2 \ln x - 2b^2 \ln s - x^2 + s^2}{4D} \tag{2.97}
\]

The mean of \( W \) over all starting points in the annular space, which is the mean time to capture, i.e., \( \tau \), can be given as

\[
\tau = \frac{1}{\pi(b^2 - s^2)} \int_{s}^{b} 2\pi x W(x) dx \tag{2.98}
\]

\[
= \frac{b^4}{2D(b^2 - s^2)} \ln \frac{b}{s} - \frac{3b^2 - s^2}{8D} \tag{2.99}
\]

In addition to this, for a spherical absorber of radius \( a \) in a spherical vessel of radius \( b \), \( W(x) \) is

\[
W(x) = \frac{2b^3/a - 2b^3/x + a^2 - x^2}{6D} \tag{2.100}
\]

which leads to the mean time to capture [11]

\[
\tau = \frac{b^6}{3Da(b^3 - a^3)} \left( 1 - \frac{9a}{5b} + \frac{a^3}{b^3} - \frac{a^6}{5b^6} \right) \tag{2.101}
\]

In the next subsection, the expressions for the accuracies of the concentration and gradient sensing performed by the RN are derived.
2.4.4 Accuracy of Concentration Sensing with a Perfectly Absorbing Sphere and a Perfectly Monitoring Sphere

In (2.79), the molecule absorption rate of RN (a spherical perfect absorber with radius \( a \)), i.e., \( I_0 = 4\pi DaC_0 \), has been derived. This deterministic rate reflects the average number of molecules which the RN absorbs per unit time. It also allows RN to sense and follow the concentration change around it. However, due to the random nature of molecular motion, there is always an uncertainty in the concentration sensing. Let us assume that the RN absorbs the molecules hitting its surface during the time \( T \). Then, the average number of molecules absorbed in time \( T \), i.e., \( R \), is

\[
R = I_0 T = 4\pi DaC_0 T
\]

(2.102)

Since the molecules are independent, \( R \) is Poisson distributed and its variance is equal to its mean, i.e., \( \langle (\delta R)^2 \rangle = \langle R \rangle \), where the brackets indicate average. Hence, the RN has a concentration measurement uncertainty given as [18]

\[
\frac{\langle (\delta C_0)^2 \rangle}{C_0^2} = \frac{\langle (\delta R)^2 \rangle}{\langle R \rangle^2} = \frac{1}{4\pi DaC_0 T}
\]

(2.103)

Now, rather than the perfectly absorbing sphere assumption, let us assume that the RN is a perfectly monitoring sphere which averages several statistically independent measurements of the number of molecules inside its volume in order to improve the measurement accuracy [11]. Let \( m(t) \) be the outputs of RN which contains all the information about the ambient concentration \( C_0 \). Using \( m(t) \), the best estimate of \( C_0 \) is [11]

\[
C_0 = \frac{3m_T}{4\pi a^3}
\]

(2.104)

where \( m_T \) is the average of \( m(t) \) over the observation time \( T \) and can be given as

\[
m_T = \frac{1}{T} \int_{t_1}^{t_1+T} m(t)dt.
\]

(2.105)

Let us assume that this estimate is repeated many times starting at widely separated times \( t_k \), \( k \in \{1, 2, \ldots\} \). The accuracy of this estimate clearly depends on how \( m_T \) fluctuates. The mean-square fluctuation of \( m_T \) is \( \langle m_T^2 \rangle - \langle m_T \rangle^2 \), where the brackets indicate an average over a large number of independent runs. The average of the \( m_T \)'s, \( \langle m_T \rangle \), is

\[
\langle m_T \rangle = \frac{4\pi a^3 C_0}{3}.
\]

(2.106)
Furthermore, \( m_T^2 \) can be also expressed as

\[
m_T^2 = \frac{1}{T^2} \int_{t_1}^{t_1+T} dt' \int_{t_1}^{t_1+T} m(t)m(t')dt'
\]

(2.107)

Let us now define the autocorrelation function \( G(\tau) \) of \( m(t) \):

\[
G(\tau) = \langle m(t)m(t+\tau) \rangle
\]

(2.108)

Note that \( G(\tau) \) is an even function of \( \tau \), that is, \( G(\tau) = G(-\tau) \). Using (2.107) and \( G(\tau) \), \( \langle m_T^2 \rangle \) can be written as

\[
\langle m_T^2 \rangle = \frac{1}{T^2} \int_0^T dt' \int_0^T G(t'-t)dt'
\]

(2.109)

Hence, the determination of \( \langle m_T^2 \rangle \) requires \( G(\tau) \). In order to find \( G(\tau) \), let us consider a large number \( B \) of molecules confined to a spherical volume of radius \( O \gg a \) including the RN with radius \( a \). Let \( w_j(t) \) be the function which is 1 if molecule \( j \) is inside the RN at time \( t \) and 0 if it is not. Hence, \( \langle w_j \rangle = a^3/O^3 \) and \( G(\tau) \) can be given by

\[
G(\tau) = \langle m(t)m(t+\tau) \rangle = \langle \sum_{j=1}^{B} w_j(t)w_j(t+\tau) \rangle + \left( \sum_{j \neq i=1}^{B} \sum_{i}^{B} w_j(t)w_i(t+\tau) \right) \]

(2.110)

Here, \( \langle w_j \rangle \) can be approximated as \( a^3/O^3 \). Due to the independence of \( w_j \) and \( w_i \), the average of double sum [second term of (2.110)] including \( B(B-1) \) terms is equal to \( B(B-1)a^6/O^6 \) or \( (Ba^3/O^3)^2 \) for the case of very large \( B \). The first term of (2.110) can be given as \( B(a^3/O^3)u(\tau) \), where \( u(\tau) \) is the probability that if a certain molecule is in the RN at time \( t \), it will be found inside the RN at the later time \( t+\tau \). Then, \( G(\tau) \) reduces to

\[
G(\tau) = \langle m(t)m(t+\tau) \rangle = Ba^3/O^3u(\tau) + \left( \frac{Ba^3}{O^3} \right)^2
\]

(2.111)

By setting \( \langle m \rangle \) as \( \langle m \rangle = \frac{Ba^3}{O^3} \), \( G(\tau) \) can be rewritten as

\[
G(\tau) = \langle m \rangle u(\tau) + \langle m \rangle^2
\]

(2.112)

Based on \( u(\tau) \), let us define the characteristic time \( \tau_0 \) as

\[
\tau_0 = \int_0^\infty u(\tau)d\tau
\]

(2.113)
and using $\tau_0$ and assuming $T >> \tau_0$, the integration used for finding $\langle m_T^2 \rangle$ in (2.109) can be approximated as [11]

$$\langle m_T^2 \rangle = \frac{1}{T^2} \int_0^T dt' \left( T \langle m \rangle^2 + 2 \tau_0 \langle m \rangle \right)$$

$$= \langle m_T \rangle^2 + \frac{2\tau_0}{T} \langle m_T \rangle$$

(2.114)

Hence, the mean-square fluctuation of $m_T$, i.e., $\langle (\delta m_T)^2 \rangle$, is

$$\langle (\delta m_T)^2 \rangle = \langle m_T^2 \rangle - \langle m_T \rangle^2$$

$$= \frac{2\tau_0}{T} \langle m_T \rangle$$

(2.115)

Using the solution of diffusion equation defined in (2.53) and some electrical analogy, $\tau_0$ can be derived as

$$\tau_0 = \frac{2a^2}{5D}$$

(2.116)

For the details of the derivation, see [11]. Now, by substituting $\tau_0$ and $\langle m_T \rangle$ into (2.106), the mean-square fluctuation of $m_T$ becomes

$$\langle (\delta m_T)^2 \rangle = \langle m_T^2 \rangle - \langle m_T \rangle^2$$

$$= \left( \frac{4a^2}{5DT} \right) \langle m_T \rangle$$

(2.117)

Hence, finally, the concentration measurement uncertainty of RN, which is assumed to be a perfectly monitoring sphere, can be found as

$$\frac{\langle (\delta C_0)^2 \rangle}{C_0^2} = \frac{\langle (\delta m_T)^2 \rangle}{\langle m_T \rangle^2} = \frac{\langle m_T^2 \rangle - \langle m_T \rangle^2}{\langle m_T \rangle^2} = \frac{3}{5\pi T D C_0 a}$$

(2.118)

Note that the concentration measurement uncertainty for the case in which the RN is a perfectly absorbing sphere is actually smaller than the case of a perfectly monitoring sphere. This clearly stems from the fact that the perfectly absorbing sphere is assumed to remove particles from the environment, and thus, it does not measure the same particle more than once [18]. Next, the accuracies of gradient sensing with perfectly absorbing and monitoring spheres are introduced.
2.4.5 Accuracy of Gradient Sensing with Perfectly Absorbing and Perfectly Monitoring Spheres

In addition to the measurement of a constant concentration, the receiver nanomachine (RN) can also measure a local gradient of molecules which is generated by the transmitter nanomachine (TN). Due to the random nature of molecular motions, such gradient measurements of RN are also subject to some uncertainties. In this subsection, these uncertainties are investigated. Let us first assume that the RN is a perfectly absorbing sphere. In such a gradient measurement, to calculate the current density $\vec{j}$, a standard analogy to electrostatics can be used. In electrostatics, the potential $\phi$ and electric field $\vec{E}$ in a charge-free environment are found by Laplace’s equation, i.e., $\nabla^2 \phi = 0$, and $\vec{E} = -\nabla \phi$, respectively. Based on this analogy, the surface charge density $\sigma_{\text{charge}}$ on a conducting sphere (boundary condition $\phi = 0$ at $r = a$) placed in an electric field of magnitude $E_z$ in the $z$-direction with an additional constant potential $\phi$ far away from the sphere is given by [25]

$$
\sigma_{\text{charge}} = -\frac{1}{4\pi} \frac{\partial \phi}{\partial r} \bigg|_{r=a} = -\frac{1}{4\pi} \left( \frac{\phi}{a} - 3E_z \cos \theta \right) \quad (2.119)
$$

where $\theta$ is the polar angle measured with respect to the $z$-axis. For the case of molecule absorption with RN, the molecule concentration $C$ and the current density $\vec{j}$ follow equations analogous to the equations governing the potential $\phi$ and electrical field $\vec{E}$ in electrostatics. In particular, the spatial dependence of the concentration $C$ follows from the diffusion equation at steady state, which means $\nabla^2 C = 0$. On the other hand, the current density is given by $\vec{j} = -D \vec{V} C$. By using (2.119), the average current density impinging on the RN (with boundary condition $C = 0$ at $r = a$) in a background gradient $C_z = \partial C / \partial z$ in the $z$-direction is given by

$$
j(\theta) = \frac{DC_0}{a} + 3DC_z \cos \theta \quad (2.120)
$$

where $C_0$ is a constant background concentration. Equation (2.120) can be also generalized to a gradient $\vec{V} C$ in an arbitrary direction $\vec{r}$ as follows:

$$
j(\theta, \phi) = \frac{DC_0}{a} + 3D \vec{V} C \cdot \vec{e}(\theta, \phi) \quad (2.121)
$$

where $\vec{e}(\theta, \phi) = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta)$. In order to estimate the molecule gradient from an observed density of molecules (the observation is based on the molecule absorption of RN) during time $T$, it is possible to fit the observed density

$$
\sigma_{\text{obs}}(\vec{r}) = \sum_{i=1}^{U} \delta(\vec{r} - \vec{r}_i) \quad (2.122)
$$
to the expected density \( j(\theta, \phi)T \) from (2.121). Here, \( U \) is the total number of absorbed molecules and \( \delta(\cdot) \) is the Dirac delta function. The best fit can be attained by minimizing the error between the observed density and the expected density, which is given by

\[
\text{Error} = \int \left[ \sigma^\text{obs}_T - H - \sum_{m=-1,0,1} G_m Y^m_{l=1}(\theta, \phi) \right]^2 dA
\]  
(2.123)

where the expected contribution from the gradient is given in terms of the spherical harmonics \( Y^m_{l=1}(\theta, \phi) \), i.e.,

\[
Y^{-1}_{1} = \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi}, \quad Y^{0}_{1} = \sqrt{\frac{3}{4\pi}} \cos \theta, \quad Y^{1}_{1} = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}. \tag{2.124}
\]

Furthermore, in (2.123), \( H \) and \( G_m (m = -1, 0, 1) \) are the parameters which need to be identified. The minimization of the error as a function of the parameters \( H \) and \( G_m \) can be achieved through \( \partial \text{Error} / \partial H = 0 \) and \( \partial \text{Error} / \partial G_m = 0 \). Hence, this yields the best fit values:

\[
H = \frac{\int \sigma^\text{obs}_T dA}{\int dA} = \frac{\int \sigma^\text{obs}_T dA}{4\pi a^2}
\]  
(2.125)

\[
G_{-1} = \frac{\int \sigma^\text{obs}_T Y^{-1}_{1}(\theta, \phi) dA}{\int |Y^{-1}_{1}(\theta, \phi)|^2 dA} = \sqrt{\frac{3}{2\pi}} \frac{\int \sigma^\text{obs}_T \sin \theta e^{-i\phi} dA}{a^2}
\]  
(2.126)

\[
G_0 = \frac{\int \sigma^\text{obs}_T Y^{0}_{1}(\theta, \phi) dA}{\int |Y^{0}_{1}(\theta, \phi)|^2 dA} = \frac{1}{2} \sqrt{\frac{3}{2\pi}} \frac{\int \sigma^\text{obs}_T \cos \theta dA}{a^2}
\]  
(2.127)

\[
G_{1} = \frac{\int \sigma^\text{obs}_T Y^{1}_{1}(\theta, \phi) dA}{\int |Y^{1}_{1}(\theta, \phi)|^2 dA} = -\sqrt{\frac{3}{2\pi}} \frac{\int \sigma^\text{obs}_T \sin \theta e^{i\phi} dA}{a^2}
\]  
(2.128)

Then, the best estimates of the background concentration and the individual gradient components can be given as

\[
C_0 = \frac{aH}{DT}
\]  
(2.129)

\[
C_x = \frac{1}{6DT} \sqrt{\frac{3}{2\pi}} (G_{-1} - G_{1})
\]  
(2.130)

\[
C_y = -\frac{i}{6DT} \sqrt{\frac{3}{2\pi}} (G_{1} + G_{-1})
\]  
(2.131)

\[
C_z = \frac{1}{6DT} \sqrt{\frac{3}{\pi}} G_0
\]  
(2.132)
The gradients estimates $C_{x,y,z}$ are the independent and orthogonal components of the gradient. Without loss of generality, let us first consider only the gradient estimate in the $z$-direction. Using (2.132), the best estimates of the gradient in the $z$-direction after absorption of molecules during $T$ can be computed as follows.

$$C_z = \frac{\int \sigma_T^{\text{obs}} \cos \theta dA}{4\pi Da^2 T} = \frac{\sum_{i=1}^U \cos \theta_i}{4\pi Da^2 T}$$

(2.133)

Based on (2.133), the gradient measurement uncertainty of RN can be identified through the variance of $C_z$, i.e., $\langle (\delta C_z)^2 \rangle$, given by

$$\langle (\delta C_z)^2 \rangle = \langle C_z^2 \rangle - \langle C_z \rangle^2$$

$$= \frac{\langle \sum_{i=1}^U \cos^2 \theta \rangle + \langle \sum_{i=1}^U \sum_{i \neq j}^U \cos \theta_i \cos \theta_j \rangle}{(4\pi Da^2 T)^2} - \frac{\langle \sum_{i=1}^U \cos \theta_i \rangle^2}{(4\pi Da^2 T)^2}$$

$$= \frac{\langle \sum_{i=1}^U \cos^2 \theta \rangle}{(4\pi Da^2 T)^2} = \frac{\langle U \rangle \langle \cos^2 \theta \rangle}{(4\pi Da^2 T)^2}$$

$$= \frac{C_0}{12\pi Da^3 T}$$

(2.134)

Note that in the derivation given above, since $U$ is Poisson distributed and the molecules are independent, $\langle \sum_{i=1}^U \sum_{i \neq j}^U \cos \theta_i \cos \theta_j \rangle$ is set to $\langle U (U - 1) \rangle \langle \cos \theta \rangle^2 = \langle U \rangle^2 \langle \cos \theta \rangle^2$. The approximation is based on the assumption that $U$ is a very large value. Furthermore, $\langle U \rangle$ and $\langle \cos^2 \theta \rangle$ are set to $\langle U \rangle = 4\pi Da C_0 T$ and $\langle \cos^2 \theta \rangle = 1/3$, respectively. Since the gradient may come from an arbitrary direction, the total gradient measurement uncertainty can be normalized by $C_0/a$ and written as [18]

$$\frac{\langle (\delta C_z)^2 \rangle}{(C_0/a)^2} = \frac{3 \langle (\delta C_z)^2 \rangle}{(C_0/a)^2} = \frac{1}{4\pi Da C_0 T}$$

(2.135)

where the factor 3 stems from the fact that each component of the gradient (i.e., $C_x$, $C_y$, and $C_z$) contributes independently to the total uncertainty. Notice also that the concentration measurement uncertainty of the perfectly absorbing RN in (2.103) and the gradient sensing uncertainty of the perfectly absorbing RN in (2.135) are the same. This reveals that the gradient sensing uncertainty of a perfectly absorbing RN is independent of the magnitude of the gradient (including the case of no gradient).

Now, let us assume that RN is a perfectly monitoring sphere which averages several statistically independent measurements of the number of molecules inside its volume in order to improve the accuracy of the measurement [11].
The concentration measurement uncertainty of a perfectly monitoring RN has been given in (2.118). In the following, the gradient sensing uncertainty of the perfectly monitoring RN is derived. To this end, a best estimate of the gradient is first derived. Then, the variance of this best estimate to obtain the uncertainty of the gradient estimation is derived.

Let us start by fitting a gradient model \( C = C_0 + \vec{r}.\vec{C}_r \) to the observed time-averaged density obtained by measuring exact positions of the molecules inside the RN (the volume of the sphere) during \( T \), i.e.,

\[
\frac{1}{T} \int dt \rho_{\text{obs}}(t) = \frac{1}{T} \int dt \sum_{i=1}^{U} \delta(\vec{r} - \vec{r}(t)).
\] (2.136)

Note that the observed density has been denoted by \( \sigma_{T}^{\text{obs}} \) in the previous analysis of the perfectly absorbing RN. However, it is denoted by \( \rho_{\text{obs}}(t) \) in this analysis. Then, the error can be given by

\[
\text{Error} = \int \left( \frac{1}{T} \int \rho_{\text{obs}}(t) dt - C_0 - \vec{r}.\vec{C}_r \right)^2 dV
\] (2.137)

As in the previous case of the perfectly absorbing RN, let us focus on the gradient in the \( z \)-direction, i.e., \( C_z \). By using \( \partial \text{Error}/\partial C_z = 0 \), a best estimate of \( C_z \) can be obtained as

\[
C_z = \frac{\frac{1}{T} \int dt \int dV z \rho_{\text{obs}}(t)}{\int dV \frac{z^2}{2}}
\] (2.138)

Then, the variance of this estimate can be given by

\[
\langle (\delta C_z)^2 \rangle = \langle C_z^2 \rangle - \langle C_z \rangle^2
\]

\[
= \left( \frac{15}{4\pi a^5} \right)^2 \frac{1}{T^2} \left[ \langle \left( \int dt \int dV z \rho_{\text{obs}}(t) \right)^2 \rangle - \langle \left( \int dt \int dV z \rho_{\text{obs}}(t) \right) \rangle^2 \right] - \left( \frac{15}{4\pi a^5} \right)^2 \left[ \langle m_z^2,T \rangle - \langle m_z,T \rangle^2 \right]
\] (2.139)

Notice that \( \int dV z^2 = 4\pi a^5/15 \) is used in the above derivation and

\[
\langle m_z^2,T \rangle = \frac{1}{T^3} \left( \int dt \int dV \rho_{\text{obs}}(t) \right)^2 = \frac{1}{T^2} \int_0^T dt \int_0^T dt' \langle m_z(t)m_z(t') \rangle
\]

\[
\langle m_z,T \rangle = \frac{1}{T} \left( \int dt \int dV \rho_{\text{obs}}(t) \right) = \frac{1}{T} \int_0^T dt \langle m_z(t) \rangle
\] (2.140)
where \( m_z(t) \) is the sum of the \( z \)-coordinates of all molecules inside the RN at time \( t \). In order to calculate \( m_z(t) \), let assume that the RN is enclosed in a much larger volume including \( M \) molecules. Hence, \( m_z(t) \) can be expressed as \( m_z(t) = \sum_{i=1}^{M} z_i(t) \), where \( z_i \) is the \( z \)-coordinate of molecule \( i \) if this molecule is in the RN and \( z_i \) is zero if it is outside. Let us also suppose that \( N(t) \) is the number of molecules in the RN at time \( t \) and thus \( \langle N \rangle \) can be given as \( \langle N \rangle = \frac{4}{3} \pi a^3 C_0 \). Then, \( \langle m_z(t)m_z(t') \rangle \) in (2.140) can be written as

\[
\langle m_z(t)m_z(t') \rangle = \left\langle \sum_{i=1}^{M} \sum_{j=1}^{M} z_i(t)z_j(t') \rightangle
\]

\[
= \left\langle \sum_{i=1}^{M} z_i(t)z_i(t') \rightangle + \left\langle \sum_{i=1}^{M} z_i(t) \rightangle \left\langle \sum_{j \neq i}^{M} z_j(t') \rightangle
\]

\[
= \langle N \rangle \langle z(t)z(t') \rangle + \langle N \rangle^2 \langle z(t) \rangle^2
\]

\[
= \frac{4}{3} \pi a^3 C_0 s(t - t') + \langle m_z(t) \rangle^2
\]

(2.141)

where \( s(t - t') = \langle z(t)z(t') \rangle \) and \( \left\langle \sum_{j=1}^{M} z_j(t') \right\rangle \approx \left\langle \sum_{j \neq i}^{M} z_j(t') \right\rangle \) is employed under the assumption that \( M \) is very large. By substituting (2.141) and (2.140) into (2.139), the variance of the estimated gradient can be rewritten as

\[
\left\langle (\delta C_z)^2 \right\rangle = \frac{75C_0}{4\pi a^7 T^2} \int_0^T dt \int_0^T dt' s(t - t')
\]

(2.142)

For the case in which time \( T \) is much larger than the correlation time \( \tau_z \) which is defined as

\[
\tau_z = \frac{1}{\langle z(t)z(t') \rangle} \int_0^\infty d\tau s(\tau)
\]

(2.143)

the integration operation in (2.142) can be simplified. More specifically, based on the symmetry \( s(\tau) = s(-\tau) \) for equilibrium diffusion, (2.142) reduces to

\[
\left\langle (\delta C_z)^2 \right\rangle = \frac{75C_0 \tau_z}{2\pi a^5 T}
\]

(2.144)

The correlation time \( \tau_z \) can be derived as \( 2a^2/105D \). For the details of the derivation, see [18]. Hence, \( \tau_z = 2a^2/105D \) can be used in (2.144) in order to find the normalized gradient measurement uncertainty as follows:

\[
\frac{\left\langle (\delta C_z)^2 \right\rangle}{(C_0/a)^2} = \frac{5}{7\pi DaC_0 T}
\]

(2.145)
Due to the fact that each component of the gradient contributes independently, the total normalized uncertainty is finally obtained multiplying (2.145) by the factor 3 as follows:

\[
\frac{\langle (\delta C_r)^2 \rangle}{(C_0/a)^2} = \frac{15}{7\pi DaC_0 T}
\]

(2.146)

By comparing (2.135) and (2.146), it can be easily concluded that in the gradient sensing, the uncertainty of the perfectly absorbing RN is smaller than the uncertainty of the perfectly monitoring RN. Recall that in the concentration sensing, the same result was obtained. That is, the uncertainty of perfectly absorbing RN was smaller than the uncertainty of perfectly monitoring RN. The reason of this is that the perfectly absorbing sphere is assumed to remove particles from the environment, and thus, it does not measure the same particle more than once [18]. In the following section, by incorporating the molecule emission, diffusion, and reception processes introduced in Sects. 2.2–2.4, unified models are presented for PMC with perfect absorber.

### 2.5 Unified Models for PMC with Perfect Absorber

In Sects. 2.2–2.4, the models are given for the molecule emission, diffusion, and reception in PMC with perfect absorber, respectively. In this section, by incorporating these models, two unified models are introduced. The first model is based on the reaction-rate equations of the molecule emission, diffusion, and reception [4]. The second model is based on the reaction–diffusion equations.

#### 2.5.1 Unified Model with Reaction-Rate Equations

Here, the PMC between the TN and RN is assumed to include the four different phenomena called the emission of molecules, diffusion of molecules, reception of molecules, and degradation of molecules as elaborated below.

##### 2.5.1.1 Emission and Diffusion of Molecules

Let us assume that the TN emits messenger molecule \( S \) into the medium with the emission rate \( \eta(t) \). Hence, the emission of \( S \) can be characterized as follows:

\[
\ast \frac{\eta(t)}{S}
\]

(2.147)
Fig. 2.16 Illustration of the PMC between the TN and RN. The TN emits messenger molecules and they diffuse in the medium. Then, each molecule that is able to reach to the RN is received by the RN ⋆

where ⋆ denotes the sources that enable the synthesis and emission of S. Let \( X(t) \) be the number of molecule S emitted by the TN at time \( t \) and thus, \( X(t) \) can be considered as the input signal of the PMC channel. The time derivative of \( X(t) \) is

\[
\dot{X}(t) = \eta(t) \tag{2.148}
\]

and thus,

\[
X(t) = \int_0^t \eta(s) ds \tag{2.149}
\]

The fraction of the emitted molecules which are captured by the RN is

\[
\rho = \frac{a}{b} \tag{2.150}
\]

where \( a \) is the radius of TN and \( b \) is the distance between the TN and RN. Recall that (2.150) has been already derived in (2.89) in Sect. 2.4.2. Let \( \overline{S} \) denote molecule S which will be captured by the RN (see Fig. 2.16). Let \( \overline{X}(t) \) be the number of \( \overline{S} \). The number of \( \overline{S} \) is just a portion of the emitted molecules \( S \). Therefore, it can be expressed as

\[
\overline{X}(t) = \rho X(t) \tag{2.151}
\]

Due to the linear relation between \( X(t) \) and \( \overline{X}(t) \), the generation of molecules \( \overline{S} \) can be also characterized by

\[
\star \xrightarrow{\eta(t)} \overline{S} \tag{2.152}
\]

where \( \overline{\eta}(t) \) is the emission rate of molecules \( \overline{S} \) and it can be given as

\[
\overline{\eta}(t) = \rho \eta(t) \tag{2.153}
\]

Next, the molecular reception process is introduced.
2.5.1.2 Reception of Molecules

After each molecule $\overline{S}$ is emitted through (2.152), it is captured by the RN. Let $S^*$ be the received $\overline{S}$ molecule (see Fig. 2.16) and $Y(t)$ be the concentration of the molecules $S^*$ delivered to the RN and thus, $Y(t)$ can be considered as the output signal of the PMC channel. Then, the molecule reception process can be characterized by

$$\overline{S} \xrightarrow{\lambda} S^*$$  \hspace{1cm} (2.154)

where $\lambda$ is the reception rate of the molecules $\overline{S}$. $\lambda$ reflects how long it takes for a $\overline{S}$ to be captured by the RN and converted to $S^*$. Hence, $\lambda$ can be expressed as $\lambda = 1/\tau$ [40], where $\tau$ is the mean time required by the RN to capture $\overline{S}$ after it is emitted by the TN. Recall that $\tau$ has been already investigated in Sect. 2.4.3. Next, the molecular degradation process is discussed and modeled.

2.5.1.3 Degradation of Molecules

Due to some external factors such as pH or temperature level of the medium or some specific quenching enzyme, the messenger molecules may degrade.\(^4\) Hence, the molecule degradation is a part of the PMC between the TN and RN and can be characterized by

$$\overline{S} \xrightarrow{\gamma} \star$$  \hspace{1cm} (2.155)

where $\gamma$ denotes the degradation rate and $\star$ denotes that $\overline{S}$ degrades and no longer exits in the medium. If we assume that each molecule has an average lifetime, then, the degradation rate can be given as the multiplicative inverse (or reciprocal) of the average lifetime.

The reactions defined in (2.152), (2.154), and (2.155) can be combined to provide a unified deterministic model for PMC. Using the emission rate ($\eta(t)$), the reception rate ($\lambda$), and the degradation rate ($\gamma$), the time derivatives of $X(t)$ and $Y(t)$ are given by the following reaction-rate equations:

$$\dot{X}(t) = \eta(t) - (\gamma + \lambda)X(t)$$  \hspace{1cm} (2.156)

$$\dot{Y}(t) = \lambda X(t)$$  \hspace{1cm} (2.157)

Using (2.156) and (2.157), $X(t)$ and $Y(t)$ are derived for the cases of constant and time-varying emission rates. For the case of constant emission rate, the TN is assumed to emit molecule $S$ with a constant emission rate ($\eta(t) = \eta$). Then, the channel input is

\(^4\)For example, in most of the bacteria-based PMC systems (see [9]), the degradation of the messenger molecules is taken into consideration.
The emission rate $\bar{\eta}(t)$ of $S$ molecules is also constant and it is equal to $\bar{\eta} = \rho \eta$. Hence, by solving (2.156) and (2.157), $X(t)$ and the channel output $Y(t)$ can be found as

$$X(t) = \eta t$$

(2.158)

where $\alpha = (\gamma + \lambda)$. For this case, the solutions reveal interesting result that $X(t)$ and $Y(t)$ are the linear functions of the emission rate $\eta$. Hence, the channel output $Y(t)$ can be linearly decreased and increased by simply changing the emission rate $\eta$. As $\eta$ varies, the amplitude of $Y(t)$ varies while its curve shape remains the same. Such a regulation can be used to develop efficient a kind of amplitude modulation schemes for PMC.

In the case of time-varying emission rate, the TN is assumed to emit molecules $S$ with a time-varying emission rate, i.e., $\eta(t)$. Using $\eta(t)$, the channel input $X(t)$ can be found as given in (2.149). Furthermore, the emission rate of $S$ molecules is $\bar{\eta}(t) = \rho \eta(t)$. For this case, by solving (2.156) and (2.157), $X(t)$ and $Y(t)$ can be given as

$$X(t) = e^{-\alpha t} \left[ - \int_0^t e^{\alpha c} \bar{\eta}(c) dc + \int_1^t e^{\alpha c} \bar{\eta}(c) dc \right]$$

(2.160)

$$Y(t) = - \int_0^t \lambda X(a) da + \int_1^t \lambda X(a) da$$

(2.161)

Specifically, by setting $\eta(t)$ as $\eta(t) = c [1 + \sin(2\pi ft)]$, $X(t)$, $\bar{X}(t)$ and $Y(t)$ can be obtained as follows.

$$X(t) = c \left[ t + \frac{[\sin(\pi ft)]^2}{\pi f} \right]$$

(2.162)

$$\bar{X}(t) = \frac{\rho c \left[ e^{-\alpha t} [\kappa \alpha - \Gamma] + \Gamma - \kappa \alpha \cos(\kappa t) \right]}{\alpha \Gamma} + \frac{\rho c \alpha \sin(\kappa t)}{\alpha \Gamma}$$

(2.163)

$$Y(t) = \frac{e^{-\alpha t} \lambda c \rho}{\alpha^2 \Gamma \kappa} \left[ \kappa(\Gamma - \kappa \alpha) + e^{\alpha t} \left[ \alpha^3 - \Gamma \kappa + \alpha \kappa(\kappa + \Gamma t) - \alpha^2 [\alpha \cos(\kappa t) + \kappa \sin(\kappa t)] \right] \right]$$

(2.164)
Fig. 2.17 The channel input \( X(t) \) is shown with the varying frequencies \( f \) of the sinusoidal emission rate \( \eta(t) \).

Fig. 2.18 The channel output \( Y(t) \) is shown with the varying frequencies \( f \) of the sinusoidal emission rate \( \eta(t) \).

where \( \kappa = 2\pi f \) and \( \Gamma = (\alpha^2 + \kappa^2) \). In Figs. 2.17 and 2.18, \( X(t) \) and \( Y(t) \) are shown using the sinusoidal emission rate \( \eta(t) = 0.002[1 + \sin(2\pi ft)] \) with the different values of \( f \) and setting \( b = 0.3 \) cm. The channel output \( Y(t) \) follows the same sinusoidal pattern with \( X(t) \) as \( f \) changes. Furthermore, the frequency of \( Y(t) \) is almost the same with the frequency of \( X(t) \). This attribute of PMC can be clearly employed to develop a kind of frequency modulation scheme to carry the information by regulating the frequency of the input signal. In addition to the sinusoidal emission rate, for an exponential emission rate, i.e., \( \eta(t) = e^{-mt} \), \( X(t) \), \( \overline{X}(t) \) and \( Y(t) \) are

\[
X(t) = \frac{1 - e^{-nt}}{n} \\
\overline{X}(t) = \frac{\rho[e^{-mt} - e^{-\alpha t}]}{\alpha - n}
\] (2.165) (2.166)
\[ Y(t) = \frac{\rho \lambda \left[ \alpha (1 - e^{-\alpha t}) + n (e^{-\alpha t} - 1) \right]}{\alpha n (\alpha - n)} \] (2.167)

In addition to the deterministic models introduced above, it is also possible to derive a probabilistic model for PMC by using the similar approach followed in deriving the deterministic model. Let us recall and rewrite the molecule emission, reception, and degradation processes given in (2.152), (2.154), and (2.155):

**Emission**: \[ \star \overset{\eta}{\rightarrow} S \] (2.168)

**Reception**: \[ S \overset{\lambda}{\rightarrow} S^* \] (2.169)

**Degradation**: \[ S \overset{\gamma}{\rightarrow} \star \] (2.170)

Let \( x_1 \) and \( x_2 \) denote the number of molecules \( S \) and \( S^* \), respectively. Then, the time derivative of \( x_1 \) and \( x_2 \) can be written in the following matrix form:

\[ \dot{x} = Ax + b \] (2.171)

where \( x, A \) and \( b \) are

\[ x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad A = \begin{bmatrix} -(\lambda + \gamma) & 0 \\ \lambda & 0 \end{bmatrix}, \quad b = \begin{bmatrix} \eta \\ 0 \end{bmatrix} \] (2.172)

By following the theory introduced in [26], the probability distribution \( P(t, x) \) can be given by

\[ P(t, x) = \mathcal{P}(x, \nu(t)) * \mathcal{M}(x, \delta_1, p^{(1)}(t)) * \mathcal{M}(x, \delta_2, p^{(2)}(t)) \] (2.173)

where \( * \) denotes the convolution operation. \( \delta_1 \) and \( \delta_2 \) are the initial concentration (i.e., number) of molecules \( S \) and \( S^* \), respectively, i.e., \( x_1(0) = \delta_1 \) and \( x_2(0) = \delta_2 \). \( \mathcal{P}(x, \nu(t)) \) and \( \mathcal{M}(x, \delta_i, p^{(i)}(t)), i \in \{1, 2\} \) are the product Poisson and the multinomial (or polynomial) distributions, respectively. The vectors \( \nu(t) \in \mathbb{R}^2 \) and \( p^{(i)}(t) \in [0, 1]^2 \) are the solutions of the following reaction-rate equations:

\[ \dot{\nu}(t) = A \nu(t) + b, \quad \nu(0) = 0 \] (2.174)

\[ \dot{p}^{(i)}(t) = A p^{(i)}(t), \quad p^{(i)}(0) = \varepsilon_i \] (2.175)

where \( \varepsilon_i \) denotes the \( i \)th column of the identity matrix in \( \mathbb{R}^{2 \times 2} \) and \( 0 \) is the zero vector in \( \mathbb{R}^2 \). If it is assumed that initially there is no molecule \( S \) and \( S^* \), which means \( x_1(0) = \delta_1 = 0 \) and \( x_2(0) = \delta_2 = 0 \), then the multinomial distributions in (2.173) become
Fig. 2.19 $P(t,x)$ in (2.177) is shown with changing values of $x_1$ and $x_2$ for $t=1,500$ s.

\[ \mathcal{M}(x, 0, p^{(1)}(t)) = 1, \quad \mathcal{M}(x, 0, p^{(2)}(t)) = 1 \] (2.176)

and $P(t, x)$ reduces to

\[ P(t, x) = \mathcal{P}(x, \nu(t)) \] (2.177)
\[ = \frac{\nu_1^{x_1}}{x_1!} \times \frac{\nu_2^{x_2}}{x_2!} \times e^{-|\nu|} \] (2.178)

where $|\nu| = \sum_{i=1}^{2} |\nu_i|$. Note that for the ease of illustration, the time dependency of $\nu_i(t)$ is neglected (i.e., $\nu_i = \nu_i(t)$). By solving (2.174), $\nu_1(t)$ and $\nu_2(t)$ can be given as follows:

\[ \nu_1(t) = \frac{\rho \eta (1 - e^{-\alpha t})}{\alpha} \]
\[ \nu_2(t) = \frac{e^{-\alpha t} \rho \eta \lambda \left[ 1 + e^{\alpha t} (\alpha t - 1) \right]}{\alpha^2} \] (2.179)

where $\alpha = (\gamma + \lambda)$. Note that $\nu_1(t)$ and $\nu_2(t)$ are the same with $\bar{X}(t)$ and $Y(t)$ given in (2.159). This is the inherent connection between the deterministic and probabilistic models. In Fig. 2.19, $P(t, x)$ is plotted with changing values of $x_1$ and $x_2$ for $t=1,500$ s. Molecules $S^*$ are the received molecules and thus, $x_2(t)$ can be considered as the channel output signal. By using $P(t, x)$, the marginal distribution of the channel output $x_2$, i.e., $P_2(t, x_2)$, can be given by [26]
Fig. 2.20 $P_2(t,x_2)$ in (2.180) is shown with changing values of $x_2$ for the different values of $t$.

\[ P_2(t,x_2) = \frac{v_2^x}{x_2!} e^{-|v_2|} \quad (2.180) \]

In Fig. 2.20, it can be observed how $P_2(t,x_2)$ evolves as $x_2$ and time change. By following a similar approach, background noise signal can be also modeled. Let us assume that there is a background molecule concentration in the medium and the RN receives some of these background molecules in addition to the molecules emitted by the TN. The reception of these background molecules can be characterized by

\[ \star \xrightarrow{I_0} S^* \quad (2.181) \]

where $I_0$ is the reception rate of the background molecules and it has been already derived in (2.79) as $I_0 = 4\pi DaC_0$. Remember that $a$ is the radius of RN which is considered as a perfect absorber and $C_0$ is the background molecule concentration. Let $g(t)$ denote the background noise signal. Then, based on (2.181), $g(t)$ can be expressed as

\[ g(t) = I_0 t \quad (2.182) \]

Furthermore, by following the theory introduced in [26], the distribution of the background noise signal, i.e., $Q(t,z)$, is

\[ Q(t,z) = \mathcal{P}(z,g(t)) \]
\[ = \frac{g^z}{z!} e^{-|g|} \quad (2.184) \]

In the following section, the second unified model based on the reaction–diffusion equations is introduced.
2.5.2 Unified Model with Reaction–Diffusion Equations

In the previous subsection, a unified model is introduced by incorporating the molecule emission, diffusion, reception, and degradation through the reaction-rate equations. Similarly, the reaction–diffusion equations can be employed to provide a unified model for PMC. The reaction–diffusion equations physically govern how the concentration of one or more substances or molecules in a medium changes with the joint influences of chemical reactions and diffusion processes. With local chemical reactions, the substances are transformed into each other while the diffusion causes the substances to spread out over a surface in space. In PMC, degradation and emission of molecules can be viewed as chemical reactions and by modifying the diffusion equation in (2.37) to include the physical dynamics of these reactions, a reaction–diffusion equation can be developed as follows [12]:

\[
\frac{\partial}{\partial t} C(x,t) = D \frac{\partial^2}{\partial x^2} C(x,t) - \gamma C(x,t) + s(x,t) \tag{2.185}
\]

where \(C(x,t)\) is the concentration of molecules emitted by the TN as a function of one special coordinate \(x\) and time \(t\). \(s(x,t)\) refers to a general source term which is switched on at \(t = 0\) and localized at the origin:

\[
s(x,t) = \eta \delta(x) \Theta(t) \tag{2.186}
\]

where \(\eta\) can be considered as an emission rate similar to the one used in (2.147). \(\delta(\cdot)\) is the Dirac delta function and \(\Theta(\cdot)\) is the unit step function. \(\gamma\) is the degradation rate of molecules as introduced in (2.155). By combining the degradation rate \(\gamma\) and the diffusion coefficient \(D\), let us define another constant:

\[
\beta = \sqrt{\frac{\gamma}{D}} \tag{2.187}
\]

One way to obtain the solution in (2.185) is to consider taking the Fourier transform of its both sides:

\[
i \omega \tilde{C}(k, \omega) = -(Dk^2 + \gamma) \tilde{C}(k, \omega) + \tilde{s}(k, \omega) \tag{2.188}
\]

where \(\tilde{C}(k, \omega)\) and \(\tilde{s}(k, \omega)\) are the Fourier transforms of \(C(x,t)\) and \(s(x,t)\), respectively, and they can be given as

\[
\tilde{C}(k, \omega) = \int_{-\infty}^{\infty} C(x,t) e^{-i(kx-\omega t)} \, dx \, dt \tag{2.189}
\]

\[
\tilde{s}(k, \omega) = \int_{-\infty}^{\infty} s(x,t) e^{-i(kx-\omega t)} \, dx \, dt = \eta \int_{0}^{\infty} e^{i\omega t} \, dt = \frac{i\eta}{\omega} \tag{2.190}
\]
Fig. 2.21 $C(x,t)$ is plotted for the different values of time ($t$) as $x$ changes from 0 to 10.

By solving (2.188), $\tilde{C}(k,\omega)$ can be found as

$$\tilde{C}(k,\omega) = \frac{-\eta}{i\omega(i\omega + Dk^2 + \gamma)} = \frac{-\eta}{Dk^2 + \gamma} \left( \frac{1}{i\omega} - \frac{1}{i\omega + Dk^2 + \gamma} \right)$$

(2.191)

By taking the inverse Fourier transform of (2.191), the solution of (2.185) can be given by [12]

$$C(x,t) = \frac{\eta}{2\beta D} I(x,t)$$

(2.192)

where

$$I(x,t) = \left[ e^{-\beta x} - e^{-\beta x} \frac{2}{2} \text{erfc} \left( \frac{2\betaDt - x}{\sqrt{4Dt}} \right) - e^{\beta x} \frac{2}{2} \text{erfc} \left( \frac{2\betaDt + x}{\sqrt{4Dt}} \right) \right]$$

(2.193)

Figure 2.21 shows how $C(x,t)$ changes with $x$ for the different $t$ values. As $t$ increases, the number of molecules that are able to reach far location increases. This result clearly corresponds to the main results of diffusion process introduced in Sect. 2.3. Similarly, in Fig. 2.22, the time evolution of $C(x,t)$ is shown for the different values of the emission rate $\eta$. As expected, $C(x,t)$ increases with the emission rate.

In the steady state, the solution of (2.185), i.e., $C_s(x)$, can be obtained by evaluating

$$D \frac{\partial^2 C_s(x)}{\partial x^2} - \gamma C_s(x) + \eta \delta(x) = 0$$

(2.194)

and given as

$$C_s(x) = \frac{\eta}{2\beta D} e^{-\beta x}$$

(2.195)
Fig. 2.22 $C(x,t)$ is shown for the different values of $\eta$ by setting $x = 5$ and changing time from $t = 0$ to $t = 40$.

Note that for $2\beta Dt \pm x \gg \sqrt{4Dt}$, the terms with complementary error functions converge to 0 and (2.192) reduces to (2.195). In addition to this steady-state characterization, if it is assumed that molecules do not degrade or the degradation rate $\gamma$ goes to 0 ($\gamma \to 0$), then (2.185) becomes

$$\frac{\partial}{\partial t} C(x,t) = D \frac{\partial^2}{\partial x^2} C(x,t) + s(x,t)$$

(2.196)

For $s(x,t) = \eta \delta(x)\Theta(t)$ as given in (2.186), the solution of (2.196) can be provided by evaluating (2.192) for $\gamma \to 0$ as follows [12]:

$$C(x,t)|_{\gamma \to 0} = \frac{\eta}{2D} \left[ \frac{\sqrt{4Dt}}{\pi} e^{-\frac{x^2}{4Dt}} - \text{erfc} \left( \frac{x}{\sqrt{4Dt}} \right) \right]$$

(2.197)

For $s(x,t) = \eta \delta(x)\delta(t)$, (2.197) reduces to

$$C(x,t)|_{\gamma \to 0} = \frac{\eta}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

(2.198)

Notice that this solution has been already given in (2.50). Using the same setting in Fig. 2.21, $C(x,t)|_{\gamma \to 0}$ is plotted in Fig. 2.23. By comparing Figs. 2.21 and 2.23, it can be easily observed how the degradation rate $\gamma$ affects the evolution of $C(x,t)$. In the absence of the molecule degradation, more number of messenger molecules can be delivered to the RN.

Here, it is important to notice that in the literature, there is a bunch of research works [33, 36, 37] dealing with mathematically modeling the PMC. In these works, interested readers can found some other modeling approaches, which are similar to the ones introduced in this book. In the following chapter, the communication theories and techniques are introduced for PMC with perfect absorber.
2.6 Communication Theories and Techniques for PMC Through Absorbers

In this section, communication theories and techniques developed for the PMC are presented. First, two different information theoretical approaches to the PMC are given for the determination of the PMC rate. Then, the binary PMC techniques are introduced.

2.6.1 Communication Rate in PMC Through Absorbers

As in the traditional wireless communications, communication rate of a PMC channel needs to be investigated in order to deduce how fast information symbols can be communicated through messenger molecules. The calculation of this rate depends on how information is encoded using molecules. Two different approaches can be described to encode information by using molecules. In the first approach, the concentration (or number) of molecules is used to encode information and thus, in this case, the molecular channel is called as concentration channel. In the second approach, release times of molecules are used to encode information and the molecular channel is called as timing channel. In the following section, communication rate of the concentration channel is first investigated. Then, communication rate of the timing channel is discussed.
2.6.2 Communication Rate of Concentration Channel in PMC Through Absorbers

In the concentration channel approach, let us assume that the TN and RN are located in an aqueous medium as shown in Fig. 2.24. The molecules emitted by the TN diffuse in this medium and some of them collide and react with the surface of RN. Each reaction is an instantaneous event that is triggered by a collision between a molecule and the surface of RN causes an infinitesimally small pulse to allow the RN to infer the delivery of the molecule. The molecules that collide with the surface are not grasped and permanently enclosed by the RN. After the collision, the molecule is assumed to continue its free diffusion in the environment. Let us assume that the RN is encircled by a virtual reception volume (VRV), center of which is the location of RN. VRV has a unit volume and all of the interactions among the molecules and the surface of RN take place in VRV (see Fig. 2.24). Furthermore, VRV is assumed to be sufficiently small to exactly follow the physical dynamics of the reactions among molecules and the surface of RN [6].

The TN is assumed to emit the molecules $S$ with an initial concentration$^5 \times$ to the medium at time $t_0$. Note that $x$ can be considered as the input to the molecular channel. The emitted molecules start to diffuse in the medium and at time $t$, the concentration of molecules in VRV, i.e., $x_t$ can be given as

$$x_t = \frac{x}{(4\pi Dt)^{3/2}} e^{-\frac{d^2}{4Dt}}$$

$^5$Concentration of molecules ($\mu$mol/liter) can be converted to number of molecules by multiplying Avagadro constant ($6.02 \times 10^{23}$). Therefore, the number of molecules is interchangeably used for the concentration of molecules.
where $D$ is the diffusion coefficient for molecules $S$ and $d$ is the distance between the TN and RN. Note that (2.199) has been already introduced in (2.53) in Sect. 2.3.4. $x_t$ can be considered as the average number of molecules that is available and interact with the surface of RN in VRV at time $t$.

The number of reactions occurring between the molecules and the surface of RN during a time interval is actually a random variable since it is not possible to track locations and positions of all molecules. However, the probability, i.e., $a(x_t)dt$, that one reaction occurs between a molecule and the surface in the next infinitesimally small time interval $[t,t+dt]$ can be defined. In fact, $a(x_t)$ is commonly referred to as propensity function in the stochastic analysis of chemically reacting systems and also provides the logical basis for stochastic chemical kinetics in the stochastic simulation algorithms [22, 24]. $a(x_t)$ has also a special mathematical form [23] as

$$a(x_t) = px_t$$

(2.200)

where $p$ is the specific probability rate constant for the reaction among the molecules and the surface of RN in VRV and $x_t$ is the number of molecules in VRV as defined in (2.199). $pdt$ also gives the probability that a molecule randomly reacts with the surface of RN during the next $dt$. $pdt$ can be computed using the average velocity of molecules, the size of VRV, and the volume of the molecules and RN [22]. Substituting $p$ and $x_t$ given in (2.199) into (2.200), $a(x_t)$ can be written as

$$a(x_t) = \left[p e^{-\frac{d^2}{4D}}\right]^x$$

(2.201)

Let $y(t, \tau)$ be the number of reactions that occur within the time interval $[t, t+\tau]$. Using $a(x_t)$, it is possible to obtain an approximation for $y(t, \tau)$ if the following conditions can be satisfied [24]:

1. $\tau$ should be small enough, that is,

$$a(x_t) \approx a(x_{t+\tau'}) \quad \forall \ t' \in [t, t+\tau]$$

(2.202)

If (2.202) is satisfied, the rate of reactions does not significantly change in the interval $[t, t+\tau]$. With this condition, $y(t, \tau)$ can be simply considered as a Poisson random variable with the rate $\lambda = a(x_t)\tau$.

2. $\tau$ should be large enough such that the expected number of reactions in the interval $[t, t+\tau]$ should be much larger than 1, that is,

$$a(x_t)\tau >> 1$$

(2.203)

If (2.203) is satisfied, the Poisson random variable $y(t+\tau)$ can be approximated by the corresponding normal random variable $N(\lambda, \lambda)$, that is, $N(a(x_t)\tau, a(x_t)\tau)$. The normal random variable $y(t, \tau)$ given as $N(a(x_t)\tau, a(x_t)\tau)$ also can be written in the form of a standard normal random variable by using the expression:

$$N(\mu, \sigma^2) = \mu + \sigma N(0, 1)$$

(2.204)
By setting $\mu = a(x_t)\tau$ and $\sigma = \left[a(x_t)\tau\right]^{\frac{1}{2}}$ and substituting into (2.204), $y(t, \tau)$ can be expressed as

$$y(t, \tau) = a(x_t)\tau + \left[a(x_t)\tau\right]^{\frac{1}{2}}z$$  \hspace{1cm} (2.205)

where $z$ is the standard random variable $N(0, 1)$. Using the derivation of $x_t$ and $a(x_t)$, $y(t, \tau)$ can be rewritten as

$$y(t, \tau) = \left[p\tau e^{-\frac{d^2}{4Dt}x_u}\right] \frac{x}{x_u} + \left[p\tau e^{-\frac{d^2}{4Dt}x_u}x\right]^{\frac{1}{2}}z$$  \hspace{1cm} (2.206)

The concentration of emitted molecules, i.e., $x$, can be normalized into the interval $[0, 1]$ by using an upper bound $x_u$ as follows:

$$y(t, \tau) = h(t, \tau)x + \left[h(t, \tau)x\right]^{\frac{1}{2}}z$$  \hspace{1cm} (2.207)

Equation (2.207) can be also simplified as

$$y(t, \tau) = h(t, \tau)\bar{x} + \left[h(t, \tau)\bar{x}\right]^{\frac{1}{2}}z$$  \hspace{1cm} (2.208)

where $\bar{x}$ denotes the normalized $x$, i.e., $\bar{x} = \frac{x}{x_u}$, and $h(t, \tau)$ is defined as

$$h(t, \tau) = \frac{p\tau e^{-\frac{d^2}{4Dt}x_u}}{(4\pi Dt)^{3/2}}$$  \hspace{1cm} (2.209)

Clearly, (2.208) forms a model for the molecular signal received by the RN and it is similar to a Gaussian channel model in which $\bar{x}$ is the channel input, $y(t, \tau)$ is the channel output, $h(t, \tau)$ is the channel gain, and $\left[h(t, \tau)\bar{x}\right]^{\frac{1}{2}}z$ is the noise term that includes a white noise term $z$ and an input-dependent term $\left[h(t, \tau)\bar{x}\right]^{\frac{1}{2}}$. Since the channel gain $h(t, \tau)$ is a function of time, the PMC channel has time-varying characteristics. However, based on the assumption that $h(t, \tau)$ slightly changes within each $[t, t + \tau]$, the characteristics of the molecular communication channel can be investigated throughout each consecutive interval of $\tau$. Hence, in the following, communication rate of the molecular channel given in (2.208) is investigated by considering the consecutive intervals of $\tau$. Note that, in the following analysis, the normalized channel input is denoted as $x$ instead of $\bar{x}$ for ease of illustration.

Using the binary expansion of $x$ and $z$, (2.208) can be rewritten as follows: [8]

$$y(t, \tau) = 2^{\log h(t, \tau)} \sum_{i=1}^{\infty} x(i)2^{-i} + 2^{\frac{1}{2}\log h(t, \tau)}x \sum_{i=-\infty}^{\infty} z(i)2^{-i}$$  \hspace{1cm} (2.210)
where \( \log(\cdot) \) is used with base 2. By setting the peak power of the white noise term \( z \) as 1, (2.210) can be approximated as

\[
y(t, \tau) \approx 2^{n(t, \tau)} \sum_{i=1}^{\infty} x(i) 2^{-i} + 2^{k(t, \tau)} \sum_{i=1}^{\infty} z(i) 2^{-i}
\]  

(2.211)

where \([\log h(t, \tau)] = n(t, \tau)\) and \(\left\lfloor \frac{1}{2} \log h(t, \tau) x \right\rfloor = k(t, \tau)\). By further simplifying, (2.211) can be also expressed as

\[
y(t, \tau) \approx 2^{n(t, \tau) - k(t, \tau)} \sum_{i=1}^{\infty} x(i) 2^{-i} + 2^{k(t, \tau)} \sum_{i=1}^{\infty} \left[ x(i + n(t, \tau) - k(t, \tau)) + z(i) \right] 2^{-i}
\]

(2.212)

Ignoring the carry bit from the second term \( \sum_{i=1}^{\infty} \left[ x(i + n(t, \tau) - k(t, \tau)) + z(i) \right] 2^{-i} \), (2.212) approximately represents (2.210). As observed in (2.212), RN receives \([n(t, \tau) - k(t, \tau)]\) most significant bits of the input \( x \) without any noise while the rest are not seen at all due to the noise [8]. Therefore, the molecular information rate achieved in the interval \([t, t + \tau]\) in the deterministic molecular channel, i.e., \(R(t, \tau)\) (\(\text{bits}/\tau\)), can be given as

\[
R(t, \tau) = n(t, \tau) - k(t, \tau) \\
= \left\lfloor \log h(t, \tau) \right\rfloor - \left\lfloor \frac{1}{2} \log h(t, \tau) x \right\rfloor
\]

(2.213)

Figure 2.25 illustrates how \( R(t, \tau) \) evolves as the internode distance \( d \) changes. The rate \( R(t, \tau) \) decreases with \( d \). This stems from the fact that the number of molecules,
that is able to reach the close proximity of RN and received by the RN, decreases as $d$ increases. Next, communication rate of the timing channel in PMC with perfect absorber is discussed [42]. However, before passing the next section, it is important to notice that other approaches to the communication rate of the concentration channel can be found in the literature. For example, another important approach can be found in [38].

### 2.6.3 Communication Rate of Timing Channel in PMC with Perfect Absorber

In the timing channel approach, the TN is assumed to be able to control the release time and number of emitted molecules. As soon as an emitted molecule arrives at RN, the molecule is assumed to be directly absorbed by RN and does not return to the medium. Upon the arrival, RN measures the arrival time of the molecule. This also requires a time synchronization between the TN and RN. The TN transmits a message $X$ by releasing molecules into the medium, where $X \in \chi$ is a random variable with alphabet $\chi$ having a finite cardinality $|\chi|$. Let us consider a medium with positive drift velocity $v$ and diffusion coefficient $D$. If a molecule is released into the medium at time $x = 0$ at position $w = 0$, under the Wiener process, the probability density of the particle’s position $w$ at time $x > 0$, i.e., $f_W(w;x)$, is given by [28]

$$f_W(w;x) = \frac{1}{\sqrt{2\pi\sigma^2 x}} e^{-\frac{(w-vx)^2}{2\sigma^2 x}} \quad (2.214)$$

where $\sigma^2 = D/2$ and note that (2.214) is the probability density function of the position $w$ and it is Gaussian with mean $vx$ and variance $\sigma^2 x$ [42]. Let $N$ be the first arrival time. $N$ is also a random variable and for $v > 0$, its distribution, i.e., $f_N(n)$, can be expressed by the inverse Gaussian (IG) distribution [15] as follows:

$$f_N(n) = \begin{cases} \sqrt{\lambda \over 2\pi n^3} \exp \left( -\frac{\lambda(n-\mu)^2}{2\mu^2 n} \right), & n > 0, \\ 0, & n \leq 0 \end{cases} \quad (2.215)$$

where $\mu = d/v$, $\lambda = d^2/\sigma^2$ and $d$ is the distance between the TN and RN. The mean and the variance of $N$ are given by $\mu$ and $\mu^2/\lambda$, respectively. The shorthand for the IG distribution in (2.215) is IG($\mu, \lambda$), i.e., $N \sim \text{IG}(\mu, \lambda)$.

If the information is assumed to be encoded in the transmit time of each molecule, the message or the symbol alphabet is $\chi \subset \mathbb{R}_+$ and the symbol $X = x$ represents a release of a single molecule at time $x$. Suppose that a molecule is emitted at the
position 0 and it propagates via a Wiener process with drift velocity $v > 0$ and Wiener process variance $\sigma^2$ and an arrival at RN occurs at time $Y \in \mathbb{R}_+$. Then, $Y$ can be expressed as

$$Y = x + N$$  \hspace{1cm} (2.216)

where $N$ is the first arrival time of the Wiener process. Note that $Y$ is the channel output of the molecular channel since the information is encoded in the transmit time of each molecule. Let us consider an example scenario in which the message alphabet is $\chi = \{x_1, \ldots, x_t\}$ with $\Pr\{x_i\} = p_i$. If $p_i$ is set to $p_i = 1/t$, the TN can transmits up to $\log(t)$ nats per channel use. Let us assume that at time $x_i$, TN transmits message $i$. Then, RN receives the message $i$ at time $Y = x_i + N$. Note that $N$ is the random delay required by the molecule to arrive at RN. After receiving the molecule, RN computes an estimate (i.e., $\hat{X}$) of the transmitted message. If $\hat{X} = x_i$, the transmission is successful and otherwise, there is an error in the molecular communication.

The probability density of observing channel output $Y = y$ given channel input $X = x$ can be written as

$$f_{Y|X}(y|x) = \begin{cases} \frac{\sqrt{\lambda}}{2\pi(y-x)^3} \exp \left(-\frac{\lambda(y-x-\mu)^2}{2\mu^2(y-x)}\right), & y > x, \\ 0, & y \leq x. \end{cases} \hspace{1cm} (2.217)$$

As observed in (2.216), the channel is affected by the random propagation time $N$ which can be considered as an additive noise. Since the additive noise has the IG distribution, the molecular channel defined in (2.216) is called as additive inverse Gaussian noise (AIGN) Channel. AIGN channel is clearly similar to the traditional additive white Gaussian noise (AWGN) channel consisting of an input term and a noise term having white Gaussian distribution. As in the AWGN case, the mutual information between the channel input $X$ and the output $Y$ in the AIGN channel, i.e., $I(X;Y)$, can be written as

$$I(X;Y) = h(Y) - h(Y|X)$$

$$= h(Y) - h(X+N|X)$$

$$= h(Y) - h(N|X)$$ \hspace{1cm} (2.218)

Assuming that $X$ and $N$ are statistically independent from each other, $I(X;Y)$ can be also reduced to

$$I(X;Y) = h(Y) - h(N)$$ \hspace{1cm} (2.219)

where $h(Y)$ and $h(N)$ denote the differential entropy of the random variables $Y$ and $N$, respectively. Note that the differential entropy of the IG distribution with parameters $\mu$ and $\lambda$, i.e., $h_{IG(\mu,\lambda)}$, is given by [42]
2.6 Communication Theories and Techniques for PMC Through Absorbers

\[
h_{\text{IG}(\mu, \lambda)} = \log \left(2K_{-1/2}(\lambda/\mu)\mu\right) + \frac{3}{2} \frac{\partial}{\partial \gamma} K_{\gamma}(\lambda/\mu) \mid_{\gamma=-1/2} + \frac{\lambda}{2\mu} K_{1/2}(\lambda/\mu) + K_{-3/2}(\lambda/\mu) + K_{-1/2}(\lambda/\mu) \tag{2.220}
\]

where \(K_{\gamma}(.)\) is the order-\(\gamma\) modified Bessel function of the second kind. Note also that \(h(N) = h_{\text{IG}(\mu, \lambda)}\) due to the fact that the noise term \(N\) has the IG distribution with parameters \(\mu\) and \(\lambda\).

The capacity of the AIGN channel is the maximum mutual information, which can be found by maximizing the mutual information \(I(X;Y)\) over all possible input distributions \(f_X(x)\). The set of these input distributions is mostly subject to the application-dependent constraints on the input signal such as peak-constrained or mean-constrained input. Here, a mean constraint on the input signal is considered as follows:

\[E[X] \leq m. \tag{2.221}\]

In other words, (2.221) also means that the TN can wait \(m\) second on average to transmit the input signal. Based on this constraint, the capacity of the AIGN channel, i.e., \(C\), can be given as

\[
C = \max_{f_X(x):E[X]\leq m} I(X;Y) = \max_{f_X(x):E[X]\leq m} h(Y) - h_{\text{IG}(\mu, \lambda)} \tag{2.222}
\]

As seen in (2.220), \(h_{\text{IG}(\mu, \lambda)}\) is independent of \(f_X(x)\), \(C\) given in (2.222) reduces to

\[
C = -h_{\text{IG}(\mu, \lambda)} + \max_{f_X(x):E[X]\leq m} h(Y) \tag{2.223}
\]

Since the channel input \(X\) and the IG-distributed first arrival time \(N\) are nonnegative and \(Y\) is also nonnegative and \(E[Y] \leq m + \mu\). Note that \(\mu\) is the mean of \(N\) having IG distribution, i.e., \(IG(\mu, \lambda)\), and \(m\) is the upper bound for the mean of the input signal, i.e., \(E[X] \leq m\). The maximum-entropy distribution of a nonnegative random variable with a mean constraint is the exponential distribution whose parameter is the upper bound of the mean [16]. For the channel output \(Y\) having the constraint, \(E[Y] \leq m + \mu\), the maximum-entropy distribution is exponential and the maximum entropy for \(Y\) is \(\log((m+\mu)e)\). In other words, the entropy of \(h(Y)\) satisfies

\[
\max_{f_X(x):E[X]\leq m} h(Y) \leq \log((\mu+m)e) \tag{2.224}
\]

Using this upper bound of \(h(Y)\) in (2.224) and (2.223), an upper bound for the capacity of AIGN channel can be given as

\[
C \leq \log((\mu+m)e) - h_{\text{IG}(\mu, \lambda)} \tag{2.225}
\]
The capacity of AIGN channel in (2.225) is based on a constraint on mean waiting time as introduced in (2.221). However, if the mean is only constrained, the maximum waiting time is unlimited. Therefore, a peak constraint on the waiting time can be included to provide a more practical version of the AIGN channel. In this peak-constrained AIGN (PCAIGN) channel, there is some maximum waiting time $T$, at which RN is required to make a decision on its observation. Similar to the capacity of AIGN channel, the capacity of the PCAIGN can be found by solving $C = \max I(X;Y) = h(Y) - h(Y|X)$. In this expression, the term $h(Y|X)$ represents the uncertainty in the noise given the input. Therefore, $h(Y|X)$ is intuitively equal to the entropy in the noise $h(N)$. However, in the PCAIGN channel, the noise $n$ is constrained as $n \leq T$. Hence, in order to calculate the capacity of PCAIGN channel, the computation of $h(N|n \leq T)$ is required rather than $h(N)$. See [41] for the details of the derivation.

### 2.6.4 Binary Modulation in PMC Through Absorbers

In the previous sections, the PMC rate is investigated by considering the PMC channel as the concentration channel and the timing channel. However, these previous discussions do not take into account which PMC technique can be employed in order to efficiently transmit and receive molecular information. As in the traditional communication paradigms, binary modulation is one of the most potential modulation techniques in PMC. Here, three different binary PMC schemes are introduced. In the first scheme, the emission and reception of a single messenger molecule are used to communicate binary symbols, i.e., 0 and 1. In the second scheme, more than one molecules are used to send and receive binary symbols. In the third scheme, two distinct types of molecules are employed to communicate binary symbols. Next, these three schemes are elaborated.

### 2.6.5 Binary Modulation Based on Single Molecule

A binary modulation scheme in which the TN emits a single molecule in order to transmit bit 1 at the beginning of the slot duration $\tau$ is considered [5]. The bit 1 is assumed to be successfully delivered if the RN receives the molecule during $\tau$. For the transmission of bit 0, the TN emits no molecule and it is assumed to be successfully delivered if the RN does not receive any molecule during $\tau$. Otherwise, the current transmission is assumed to be unsuccessful. In Fig. 2.26, a timing diagram for this binary PMC scheme is shown. The delay $t$ experienced

---

6The TN and RN are assumed to synchronize with each other to emit and receive each molecule within the fixed duration time slots.
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Fig. 2.26 A timing diagram of the binary PMC scheme between the TN and the RN. One successful bit 1 and one erroneous bit 1 are illustrated by any molecule to reach the RN is assumed to follow the probability density function [28]:

\[ f(t) = \frac{d}{\sqrt{4\pi D t^3}} e^{-\frac{d^2}{4Dt}}, \quad t > 0 \]  

(2.226)

where \( D \) is the diffusion coefficient of the molecules and \( d \) is the distance between the TN and the RN. Note that (2.226) has been already given in (2.57). The associated cumulative distribution function of the density function \( f(t) \) (i.e., \( F(t) \)) is

\[ F(t) = \text{erfc} \left[ \frac{d}{2\sqrt{Dt}} \right], \quad t > 0. \]  

(2.227)

Suppose that the TN transmits 1 at slot \( n \) with the channel transmission probability \( \beta_n \) or transmits 0 with the probability \( (1 - \beta_n) \). Thus, the channel input at slot \( n \), i.e., \( X_n \), is \( X_n \sim \text{Bernoulli}(\beta_n), \forall n \in \{1,2,\ldots\} \). Let us first focus on the molecule emitted at slot \( n \). For the case of \( X_n = 1 \), the successful reception probability of RN (i.e., \( \alpha_n \)) is

\[ \alpha_n = \beta_n F(\tau) \]  

(2.228)

The probability that the emitted molecule cannot reach the RN within slot \( n \) (i.e., \( \xi_n \)), which means bit 1 cannot be delivered successfully, is

\[ \xi_n = \beta_n (1 - F(\tau)) \]  

(2.229)

For the case of \( X_n = 0 \), the probability of the successful delivery of 0 (i.e., \( \zeta_n \)) is

\[ \zeta_n = (1 - \beta_n) \]  

(2.230)

\(^7\)Here, \( f(t) \) is the probability density function belonging to the delay of one-dimensional motion of molecules. However, the given analyses can be directly applicable to two- and three-dimensional motion with appropriate probability density functions.
Hence, during slot \( n \), the RN receives 1 with \( \alpha_n \) and receives 0 with \( \xi_n + \zeta_n = (1 - \alpha_n) \) during slot \( n \). This can be also characterized by a Bernoulli random variable, i.e., \( G_n \sim Bernoulli(\alpha_n) \). Besides the molecule emitted at slot \( n \), the molecules, which have been transmitted for the previous \( n - 1 \) slot duration and have not been received by RN, may reach the RN. Let us assume that a molecule which has been emitted at slot \( k \in \{1, 2, \ldots, n - 1\} \) with probability \( \beta_k \) and has not been received by the RN. The probability that this molecule reach the RN at slot \( n \) (i.e., \( \lambda_{nk} \)) is

\[
\lambda_{nk} = \beta_k \left[ F((n-k+1)\tau) - F((n-k)\tau) \right], \quad k < n \tag{2.231}
\]

The probability that the molecule emitted at slot \( k \) is not received by the RN during slot \( n \) is \( (1 - \lambda_{nk}) \). In fact, the effect of such a late molecule can be viewed as a noise term and characterized by a Bernoulli random variable, i.e., \( \Gamma_{n,k} \sim Bernoulli(\lambda_{nk}) \), where \( k \in \{1, \ldots, (n - 1)\} \). Note that each \( \Gamma_{n,k} \) is independent of each other and \( \Gamma_{n,k}, \forall k \) and \( G_n \) are independent as illustrated in Fig. 2.27. Hence, total noise at slot \( n \), i.e., \( Z_n \), can be expressed by combining all of these noise terms as follows:

\[
Z_n = \sum_{k=1}^{n-1} \Gamma_{n,k} \tag{2.232}
\]

The channel output at slot \( n \), i.e., \( Y_n \), can be defined by adding the input term \( G_n \) and the noise term \( Z_n \) as \( Y_n = G_n + Z_n \). Since \( Y_n \) and \( Z_n \) are the sum of Bernoulli random variables with ranges \( \{0, 1, 2, \ldots, n\} \) and \( \{0, 1, 2, \ldots, n - 1\} \), respectively, they are described by two Poisson-Binomial random variables with the following probability mass functions (PMFs), respectively:

\[
p_i = \sum_{A \in \mathcal{A}_i} \prod_{k \in A} \lambda_{nk} \prod_{j \in A^c} (1 - \lambda_{nj}) \tag{2.233}
\]

\[
q_i = \sum_{B \in \mathcal{B}_i} \prod_{l \in B} \lambda_{ml} \prod_{m \in B^c} (1 - \lambda_{mm}) \tag{2.234}
\]

where \( Pr(Y_n = i) = p_i, i \in \{0, 1, \ldots, n\} \) and \( Pr(Z_n = i) = q_i, i \in \{0, 1, \ldots, n - 1\} \). \( \mathcal{A}_i \) and \( \mathcal{B}_i \) are the sets including all subsets of \( i \) integers selected from \( \{1, 2, \ldots, n\} \) and \( \{1, 2, \ldots, n - 1\} \), respectively. \( A \) represents the elements of \( \mathcal{A}_i \) and \( B \) represents the elements of \( \mathcal{B}_i \) and the superscript \( c \) denotes the complement operation. The mutual information between the channel input \( X_n \) and the output \( Y_n \) is

\[
I(X_n; Y_n) = H(Y_n) - H(Y_n|X_n) = H(G_n + Z_n) - H(G_n + Z_n|X_n) \tag{2.235}
\]

Due to the fact that \( X_n \sim Bernoulli(\beta_n) \) and \( G_n \sim Bernoulli(\beta_n F(\tau)) \) and \( F(\tau) \) is a constant probability, \( G_n \) can be determined if \( X_n \) is given. As illustrated in Fig. 2.27, \( X_n \) and \( Z_n \) are independent. Hence, \( H(G_n|X_n) = 0 \) and \( H(Z_n|X_n) = H(Z_n) \) and \( I(X_n; Y_n) \) reduces to
Fig. 2.27 The generation of independent random variables $G_n$ and $Z_n$ is illustrated

\begin{align}
I(X_n;Y_n) &= H(Y_n) - H(Z_n) \\
&= - \sum_{i=0}^{n} p_i \log p_i + \sum_{i=0}^{n-1} q_i \log q_i \tag{2.236}
\end{align}

The maximum achievable rate at slot $n$, i.e., $C_n$, can be computed by

\begin{align}
C_n &= \max_{\beta_n} I(X_n;Y_n) \tag{2.237}
\end{align}

Based on the statistical dependence between $p_i$ and $q_i$ given in (2.233) and (2.234), $p_i$ can be expressed as a function of $q_i$ and $\alpha_n$ as

\begin{align}
p_i &= \alpha_n q_{i-1} + (1 - \alpha_n) q_i \\
&= q_i + \alpha_n (q_{i-1} - q_i) \\
&= q_i + \beta_n F(\tau) (q_{i-1} - q_i) \\
&= q_i + \beta_n F(\tau) r_i \tag{2.238}
\end{align}
where \( r_i = q_{i-1} - q_i \). Using \( p_i = q_i + \beta_n F(\tau) r_i \), \( \partial I_n(X_n; Y_n)/\partial \beta_n \) can be written as

\[
\frac{\partial I_n(X_n; Y_n)}{\partial \beta_n} = -\sum_{i=0}^{n} F(\tau) r_i \log [q_i + \beta_n F(\tau) r_i] - \sum_{i=0}^{n} F(\tau) r_i
\] (2.239)

Note that \( q_{-1} = q_n = 0 \) and \( r_i = q_{i-1} - q_i \) and \( \sum_{i=0}^{n} F(\tau) r_i = 0 \). Hence, (2.239) becomes

\[
\frac{\partial I_n(X_n; Y_n)}{\partial \beta_n} = -F(\tau) r_0 \log [q_0 + \beta_n F(\tau) r_0] - \sum_{i=1}^{n} F(\tau) r_i \log \left[ 1 + \frac{q_i}{\beta_n F(\tau) r_i} \right] \beta_n F(\tau) r_i
\] (2.240)

In (2.240), a tight approximation for the term \( \log \left[ 1 + \frac{q_i}{\beta_n F(\tau) r_i} \right] \) can be given by

\[
\log \left[ 1 + \frac{q_i}{\beta_n F(\tau) r_i} \right] \approx \frac{q_i}{\beta_n F(\tau) r_i} \quad \text{for} \quad \left| \frac{q_i}{\beta_n F(\tau) r_i} \right| < 0.1 \forall i
\] (2.241)

Then, (2.240) becomes

\[
\frac{\partial I_n(X_n; Y_n)}{\partial \beta_n} \approx -F(\tau) r_0 \log [q_0 + \beta_n F(\tau) r_0] - \sum_{i=1}^{n} F(\tau) r_i \left[ \log [F(\tau) r_i] + \log [\beta_n] \right] - \sum_{i=1}^{n} \frac{q_i}{\beta_n}
\] (2.242)

Due to \( \sum_{i=1}^{n} r_i = q_0 \), \( \sum_{i=1}^{n} q_i = 1 - q_0 \), and \( r_0 = -q_0 \), (2.242) can be also modified as

\[
\frac{\partial I_n(X_n; Y_n)}{\partial \beta_n} \approx -F(\tau) q_0 \left[ \log \left( 1 + \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right) \right] - \\
\frac{(1 - q_0)}{\beta_n} - \sum_{i=1}^{n} F(\tau) r_i \log [F(\tau) r_i] - F(\tau) q_0 \log \left[ \frac{1}{q_0} \right]
\] (2.243)

In (2.243), the term \( \log \left( 1 + \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right) \) can be approximated as

\[
\log \left( 1 + \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right) \approx \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \quad \text{for} \quad \left| \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right| < 0.1
\] (2.244)
Based on this approximation, (2.243) reduces to

$$
\frac{\partial I_n(X_n;Y_n)}{\partial \beta_n} \approx -F(\tau) q_0 \left[ \frac{\beta_n + \beta_n F(\tau) - 1}{1 - \beta_n F(\tau)} \right] - \frac{1 - q_0}{\beta_n} - \sum_{i=1}^{n} F(\tau) r_i \log F(\tau) r_i - F(\tau) q_0 \log \left[ \frac{1}{q_0} \right]
$$

(2.245)

Then, the optimal $\beta_n$, i.e., $\hat{\beta}_n$, can be given by solving $\frac{\partial I_n(X_n;Y_n)}{\partial \beta_n} = 0$ in (2.245) as follows:

$$
\hat{\beta}_n \approx \frac{-\delta + F(\tau) - \sqrt{\left[ \delta - F(\tau) \right]^2 - 4(1 - q_0) \Sigma}}{2 \Sigma}
$$

(2.246)

where $\Sigma$ and $\delta$ are

$$
\Sigma = -\delta F(\tau) + F(\tau) q_0 + F(\tau)^2 q_0
$$

(2.247)

$$
\delta = \sum_{i=1}^{n} F(\tau) r_i \log F(\tau) r_i - F(\tau) q_0 \log(q_0)
$$

(2.248)

For $\beta_1 = 0.3$ and $\tau = 0.5$ s, in Fig. 2.28, $\hat{\beta}_n$ is plotted as the slot number changes from 1 to 20. As the internode distance $d$ changes from $d = 0.05 \mu m$ to $d = 1 \mu m$, $\hat{\beta}_n$ slightly increases and quickly converges to the optimal values. This reveals that the convergent $\hat{\beta}_n$ is used to determine the average number of bits 1 in a code word to ensure high PMC rate. Using the same setting used in Fig. 2.28, maximum achievable PMC rate, i.e., $C_n$, is shown in Fig. 2.29. The maximum achievable PMC rate changes from 0.61 to 0.69 nats/trans. or from 0.88 to 0.993 bits/trans. at slot.
As introduced in Sect. 2.5.1.3, once messenger molecules emitted by the TN, it becomes active and it is considered as a messenger whenever it is received by the RN. However, due to the pH or temperature level of the medium or some specific quenching enzyme, the messenger molecules may degrade. Now, let us assume that in the binary PMC scheme introduced above, messenger molecules degrade over time. Let \( g(u) \) be the probability density function of the molecule life expectancy (or the stability of the molecule in the environment) and be given as \( g(u) = \gamma e^{-\gamma u} \) [35]. The probability that a molecule emitted at slot \( k, \in \{1, 2, \ldots, n\} \) is received at slot \( n \) can be expressed as

\[
\hat{\lambda}_{nk} = \beta_k \int_{(n-k)\tau}^{(n-k+1)\tau} f(t) \int_{u=0}^{\infty} g(u) du dt \tag{2.249}
\]

where \( f(t) \) is the probability distribution function already introduced in (2.226). By using this probability instead of (2.231), the binary PMC scheme mentioned above can be directly applied to the same PMC scheme with the molecule lifetime assumption.
2.6.6 Binary Modulation Based on Multiple Molecules

In the binary modulation scheme introduced in the previous section, the transmission and reception of bit 0 and 1 are based on the emission and reception of a single messenger molecule. However, the emission and reception of multiple molecules can be also used to transmit and receive bits in a binary PMC scheme. Let us consider such a binary modulation scheme in which the TN emits \( N \) molecules at the beginning of the slot duration, i.e., \( \tau \), in order to transmit 1. The emitted molecules freely diffuse in the medium. Some of these molecules randomly hit the RN; thus, they are received. If the number of received molecules is more than or equal to \( m \), bit 1 is assumed to be successfully delivered to the RN as illustrated in Fig. 2.30. In order to transmit 0, the TN emits no molecule during \( \tau \). In fact, this binary PMC scheme based on multiple molecules is a simple extension of the binary PMC scheme introduced in the previous section, and it can be analyzed by following a similar approach.

Let us assume that the TN transmits 1 with the probability \( \beta \) by emitting \( N \) molecules at the beginning of the slot duration. It transmits 0 with the probability \((1 - \beta)\). During slot \( n \), the RN may receive molecules emitted at the beginning of slot \( k \), \( k \in \{1, 2, \ldots, n - 1\} \). The probability that any molecule emitted at slot \( k \) is received at slot \( n \), i.e., \( \lambda_{nk} \), is

\[
\lambda_{nk} = \beta \left( F\left( (n-k+1)\tau \right) - F\left( (n-k)\tau \right) \right) \quad k < n
\]

(2.250)

Note that \( F(\tau) \) has been already given in (2.227) and \( \lambda_{nk} \) is only available for \( k < n \); however, \( \lambda_{nn} \) can be given by \( \lambda_{nn} = \beta F(\tau) \). In fact, the number of molecules, which are emitted at slot \( k \) and received at slot \( n \), can be characterized by a random variable, i.e., \( Z_{n,k} \), which follows a binomial distribution, i.e., \( Z_{n,k} \sim Binomial(N, \lambda_{nk}) \), with the PMF:

\[
\Lambda_{n,k}(j; N, \lambda_{nk}) = \binom{N}{j} \lambda_{nk}^j (1-\lambda_{nk})^{N-j}
\]

(2.251)

Assuming that \( N \) is large enough, \( Binomial(N, \lambda_{nk}) \) can be approximated as the normal distribution \( \mathcal{N}\left(N\lambda_{nk}, N\lambda_{nk}(1-\lambda_{nk})\right) \) and thus

\[
Z_{n,k} \sim \mathcal{N}\left(N\lambda_{nk}, N\lambda_{nk}(1-\lambda_{nk})\right)
\]

(2.252)
By combining the effects of all previous slots \( k, k \in \{1, 2, \ldots, n - 1\} \), the total number of molecules received by RN during slot \( n \) can be characterized by

\[
Z_n = \sum_{k=1}^{n-1} Z_{n,k}
\]

(2.253)

Due to the linearity of the normal distribution, the distribution of \( Z_n \) is a normal distribution, i.e.,

\[
Z_n \sim \mathcal{N}(\mu_z, \sigma_z^2)
\]

(2.254)

where \( \mu_z \) and \( \sigma_z \) are

\[
\mu_z = \sum_{k=1}^{n-1} N\overline{\lambda}_{nk}, \quad \sigma_z^2 = \sum_{k=1}^{n-1} \left[ N\overline{\lambda}_{nk}(1 - \overline{\lambda}_{nk}) \right]
\]

(2.255)

\( Z_n \) can be viewed as a noise term in the PMC channel since it describes the effects of all interferences from the previous slots on the current slot (i.e., slot \( n \)). Let us assume that the TN sends bit 1 at slot \( n \) by emitting \( N \) molecules at the beginning of slot \( n \). Then, the number of molecules emitted at the beginning of slot \( n \) and received during slot \( n \) is also a random variable, i.e., \( X_n \), which follows a binomial distribution, i.e., \( X_n \sim \text{Binomial}(N, \overline{\alpha}_n) \) with the PMF:

\[
\Lambda_n(j; N, \overline{\alpha}_n) = \binom{N}{j} \overline{\alpha}_n^j(1 - \overline{\alpha}_n)^{N-j}
\]

(2.256)

where \( \overline{\alpha}_n = \overline{\lambda}_m = \beta F(\tau) \). This binomial distribution can be also approximated as a normal distribution \( \mathcal{N}(N\overline{\alpha}_n, N\overline{\alpha}_n(1 - \overline{\alpha}_n)) \) and thus

\[
X_n \sim \mathcal{N}(\mu_x, \sigma_x^2)
\]

(2.257)

where \( \mu_x \) and \( \sigma_x \) are

\[
\mu_x = N\overline{\alpha}_n, \quad \sigma_x^2 = [N\overline{\alpha}_n(1 - \overline{\alpha}_n)]
\]

(2.258)

Using \( X_n \) and \( Z_n \), for the case in which the TN sends 1 at slot \( n \), the total number of molecules received during slot \( n \), i.e., \( Y_n \), can be expressed as

\[
Y_n = X_n + Z_n
\]

(2.259)

Hence, \( Y_n \) also follows a normal distribution, i.e.,

\[
Y_n \sim \mathcal{N}(\mu_y, \sigma_y^2)
\]

(2.260)
where $\mu_y = \mu_x + \mu_z$ and $\sigma^2_y = \sigma^2_z + \sigma^2_x$. Then, for the case in which the TN emits bit 1, the probability of error, i.e., $p_e^1$, is

$$p_e^1 = \Pr(Y_n \leq m) = F_{Y_n}(m) \quad (2.261)$$

where $F_{Y_n}(\cdot)$ is the cumulative distribution of $Y_n$ and $F_{Y_n}(m)$ can be given as

$$F_{Y_n}(m) = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{m - \mu_y}{\sqrt{2\sigma^2_y}} \right) \right] \quad (2.262)$$

where erf(·) is the error function. In the case in which the TN emits bit 0, the TN emits no molecule at the beginning of slot $n$. This can be interpreted as $X_n = 0$. Therefore, in this case, $Y_n$ is equal to $Z_n$ and the probability of error, i.e., $p_e^0$, can be given as

$$p_e^0 = \Pr(Z_n > m) = 1 - F_{Z_n}(m) \quad (2.263)$$

where $F_{Z_n}(\cdot)$ is the cumulative distribution of $Z_n$ and $F_{Z_n}(m)$ can be given as

$$F_{Z_n}(m) = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{m - \mu_z}{\sqrt{2\sigma^2_z}} \right) \right] \quad (2.264)$$

The error probabilities $p_e^1$ and $p_e^0$ reflect the performance of the binary PMC scheme. They can be also used to determine the optimal values of the transmission probability $\beta$ and the threshold $m$. Furthermore, as in the binary PMC scheme introduced in the previous section, if messenger molecules are assumed to degrade over time by following the probability distribution $g(u) = \gamma e^{-\gamma u}$, the probability $\lambda_{nk}$ in (2.250) changes as

$$\tilde{\lambda}_{nk} = \beta \int_{(n-k)\tau}^{(n-k+1)\tau} f(t) \int_{t}^{\infty} g(u) du dt. \quad (2.265)$$

Then, by using $\tilde{\lambda}_{nk}$ instead of $\lambda_{nk}$ given in (2.250), the abovementioned analysis can be applied to the binary PMC scheme with molecule lifetime assumption.

### 2.6.7 M-ary Modulation Based on Different Types of Molecules

The binary modulation in PMC can be extended to an M-ary modulation scheme [21]. Let us assume that an M-ary molecular communication scheme is considered, in which $M$ different types of molecules are used and each molecule type carries a different information symbol with $u$ bits such that $M = 2^u$. Note
that for \( u = 1, M = 2 \) and the channel becomes a binary channel. In order to transmit an information symbol \( a, a \in \{1, \ldots, M\} \), the TN emits \( N \) of molecule type \( S_a, a \in \{1, \ldots, M\} \) at the beginning of the slot duration lasting for \( \tau \) seconds. The emitted molecules freely diffuse in the medium. Some of these molecules \( S_a \) randomly hit the RN; thus, they are received. If the number of received molecules \( S_a \) is more than or equal to \( m \), information symbol \( a \) is assumed to be successfully delivered to the RN. Here, the RN is assumed to be able to distinguish the \( M \) molecule types, and it can identify which type hits its surface.

Here, we consider a short-range \( M \)-ary PMC scheme in which each transmitted symbol, i.e., symbol \( 1, \ldots, M \), is interfered only by the symbol transmitted in the previous slot duration. Such an interference model can be viewed as a direct consequence of very short internode distance. Hence, if the TN transmits symbol \( a \) by emitting \( N \) of molecules \( S_a \), the RN receives some of these molecules. In addition to this, the RN may also receive some of the other \( M - 1 \) types of molecules emitted at the previous slot. For example, if symbol \( b \) was transmitted at the previous slot by emitting \( N \) molecules \( S_b \), then the RN may receive \( S_b \) molecules in addition to \( S_a \) molecules emitted at the current slot. Therefore, the delay of a transmitted symbol is affected by which symbol was transmitted at the previous slot.

For the case of symbol \( a \), there are two different cases, i.e., \( a - a \) and \( b - a \), where \( a \neq b, a \in \{1, \ldots, M\} \) and \( b \in \{1, \ldots, M\} \). Note that the first digit denotes the symbol transmitted at the previous slot and the second digit denotes the currently transmitted symbol.

**Lemma 2.1.** If the previous symbol is \( a \), the probability density function for the delay of symbol \( a \), i.e., \( f_{aa}(t) \), is

\[
 f_{aa}(t) = \frac{\sum_{j=0}^{m} \tilde{\Gamma}_j(t) \left[ \sum_{h=0}^{N-j} \tilde{\phi}_{h,j}(t) \psi_h(\tau) \right] \phi_{m-j}(t)}{\sum_{j=0}^{m} \left[ \sum_{h=0}^{N-j} \tilde{\phi}_{h,j}(t) \psi_h(\tau) \right] \phi_{m-j}(t)},
\]

(2.266)

the associated cumulative distribution function is

\[
 F_{aa}(t) = \int_0^t f_{aa}(x)dx, \quad t \geq 0
\]

(2.267)

and the associated symbol error probability (SEP), i.e., \( E_{aa} \), is \( E_{aa} = 1 - F_{aa}(\tau) \).

**Proof.** Let us assume that the current slot is slot \( n \) and the previous slot is slot \( n - 1 \) for \( n \geq 2 \). Let us define the counting process \( c(t) \), which stands for the number of molecules that have hit the RN until time \( t \), given that \( N \) molecules were emitted at the beginning of slot \( n \). The probability distribution associated with this process, i.e., \( \phi(t) \), is given by
\[
\varphi_i(t) = Pr(c(t) = i), \ i \in [0, N], \ t \geq 0 \\
= \binom{N}{i} F^i(t) [1 - F(t)]^{N-i}
\] (2.268)

Accordingly, the distribution function of the time until \(i\)th hit, given that \(N\) molecules were emitted at the beginning of slot \(n\), i.e., \(\Phi_i(t)\), can be expressed as follows:

\[
\Phi_i(t) = \sum_{\lambda=i}^{N} \varphi_\lambda(t), \ i \geq 0, \ t \geq 0 \\
= \sum_{\lambda=i}^{N} \binom{N}{\lambda} F^\lambda(t) [1 - F(t)]^{N-\lambda}
\] (2.269)

Note that in the case of \(i = 0\), \(\Phi_i(t) = 1\) for \(t \geq 0\). Let us consider a modified counting process \(\tilde{c}_h(t)\) to register the molecules that are emitted at slot \(n-1\) and hit the RN during a time interval \(t\) starting at the beginning of slot \(n\), given that \(h\) (\(0 \leq h \leq N\)) molecules have already reached the RN during slot \(n-1\). Then, the probability distribution associated with \(\tilde{c}_h(t)\) can be formulated as the probability that \(h + j\) molecules hit the RN at time \(t + \tau\) given that \(h\) molecules have already reached the RN during previous slot duration \(\tau\):

\[
\tilde{\varphi}_{h,j}(t) = Pr(\tilde{c}_h(t) = j) \\
= Pr(c(t+\tau) = h+j | c(\tau) = h) \\
= \frac{Pr(c(t+\tau) = h+j, c(\tau) = h)}{Pr(c(\tau) = h)}
\] (2.270)

The numerator of \(\tilde{\varphi}_{h,j}(t)\) in (2.270) can be expressed as

\[
Pr(c(t+\tau) = h+j, c(\tau) = h) = \binom{N}{h} \binom{N-h}{j} \times \\
\times F^h(\tau) [F(t+\tau) - F(\tau)]^j (1 - F(t+\tau))^{N-(h+j)}
\] (2.271)

The denominator of \(\tilde{\varphi}_{h,j}(t)\) can be given by \(\varphi_h(\tau)\) as it is derived in (2.268). Hence, \(\tilde{\varphi}_{h,j}(t)\) can be expressed as

\[
\tilde{\varphi}_{h,j}(t) = \binom{N-h}{j} \left[\frac{F(t+\tau) - F(\tau)}{F(\tau)}\right]^j (1 - F(t+\tau))^{N-h} (2.272)
\]
where \( r = N - (h + j) \). Similarly, the distribution function of the time until the \( j \)th hit within slot \( n \) given that \( h \) molecules already reached the RN during slot \( n - 1 \) is given by

\[
\hat{\Phi}_{h,j}(t) = \sum_{\lambda = j}^{N-h} Pr(c(t + \tau) = h + \lambda | c(\tau) = h) = \\
= \sum_{\lambda = j}^{N-h} \binom{N-h}{\lambda} \left[ F(t + \tau) - F(\tau) \right]^{\lambda} \frac{[1 - F(t + \tau)]^\delta}{[1 - F(\tau)]^{N-h}}
\tag{2.273}
\]

where \( \delta = N - (h + \lambda) \). Note that \( 0 \leq j \leq N - h \) and \( t \geq 0 \) in (2.272) and (2.273). We can now uncondition \( \hat{\Phi}_{h,j}(t) \) with regard to \( h \) by considering all possible values of \( h \):

\[
\hat{\Phi}_j(t) = \sum_{h=0}^{N-j} \hat{\Phi}_{h,j}(t) \varphi_h(\tau), \quad 0 \leq j \leq N
\tag{2.274}
\]

This is the distribution function of the time until the number of \( j \) molecules emitted at slot \( n - 1 \) hit the RN during slot \( n \). In general, during slot \( n \), a mix of molecules emitted at the beginning of slots \( n \) and \( n - 1 \) hit the RN. \( m \) is the threshold for the amount of molecules required to be received by the RN to successfully decode symbol \( a \). Hence, if the number of arrivals from slot \( n - 1 \) is \( j \), then \( m - j \) arrivals from slot \( n \) will be sufficient for the correct reception of symbol \( a \). As \( j \) changes from 0 to \( m \), there will be \( m + 1 \) different combinations of molecular arrivals from slots \( n - 1 \) and \( n \). For every combination, the time required for the RN to decide in favor of symbol \( a \) is the maximum of the hitting times experienced by the first \( m \) molecules hitting the RN and coming from slot \( n - 1 \) or \( n \). These hitting times have already been characterized in (2.269) and (2.274) and the maximum of these times is distributed according to the product of (2.269) and (2.274). Let us assume there are \( j \) arrivals from slot \( n - 1 \) and \( m - j \) arrivals from slot \( n \) and hereafter denote this combination as \((j, m - j)\). Thus, the delay distribution of the combination \((j, m - j)\), i.e., \( \Gamma_j(t) \), is the product of (2.269) and (2.274):

\[
\Gamma_j(t) = \hat{\Phi}_j(t)\Phi_{m-j}(t), \quad t \geq 0
\tag{2.275}
\]

Note that the distribution \( \Gamma_j(t) \) is available for each combination \((j, m - j), j \in \{0, \ldots, m\}\). Next, using these distributions, the distribution of the total delay experienced to successfully deliver symbol \( a \) when the previous symbol is \( a \) is derived. Let us call this delay as \( \gamma \). Then, the probability of \( t < \gamma \leq t + dt \), i.e., \( \mathcal{P} \), can be expressed as \( \mathcal{P} = f_{\text{aad}}(t)dt \), where \( f_{\text{aad}}(t) \) is the probability density function of \( \gamma \). In fact, \( \mathcal{P} \) can be also expressed as \( \mathcal{P} = \Pr(t < \gamma \leq t + dt|m \text{ hits}) \). Furthermore, by aggregating all of \( m + 1 \) combinations, i.e., \((j, m - j), j \in \{0, 1, \ldots, m\}\), \( \mathcal{P} \) can also be rewritten as
\[ \mathcal{P} = \sum_{j=0}^{m} \left[ Pr(t < \gamma < t + dt | (j,m-j)|m \text{ hits}) Pr((j,m-j)|m \text{ hits}) \right] \]  

(2.276)

In (2.276), for ease of illustration, let us denote \( Pr(t < \gamma < t + dt | (j,m-j)|m \text{ hits}) \) and \( Pr((j,m-j)|m \text{ hits}) \) as \( \eta_{j,m} \) and \( \zeta_{j,m} \), respectively. Then, using (2.275), \( \eta_{j,m} \) can be given as

\[ \eta_{j,m} = \dot{\Gamma}_{j}(t) dt \]  

(2.277)

where \( \dot{\Gamma}_{j}(t) \) is the first derivative of \( \Gamma_{j}(t) \) in (2.275) with respect to \( t \). The second term of (2.276), i.e., \( \zeta_{j,m} \), can be expressed as

\[ \zeta_{j,m} = \frac{Pr(a(t) = j)Pr(c(t) = m-j)}{\sum_{i=0}^{m} Pr(a(t) = i)Pr(c(t) = m-i)} \]  

(2.278)

where \( a(t) = [c(t+\tau) - c(\tau)] \) and \( Pr(a(t) = j) \) is

\[ Pr(a(t) = j) = \sum_{h=0}^{N-j} \left[ Pr(c(t+\tau) = h + j|c(\tau) = h) \times \right. \]

\[ \times Pr(c(\tau) = h) \right] = \sum_{h=0}^{N-j} \phi_{h,j}(t)\phi_{h}(\tau), \ t \geq 0 \]  

(2.279)

Furthermore, in (2.278), \( Pr(c(t) = m-j) = \varphi_{m-j}(t) \). Note that \( \varphi_{h}(\tau) \) and \( \bar{\varphi}_{h,j}(t) \) have been already given in (2.268) and (2.272). By substituting (2.277) and (2.278) into (2.276), \( \mathcal{P} \) can be rewritten as

\[ \mathcal{P} = \left[ \sum_{j=0}^{m} \dot{\Gamma}_{j}(t) \left[ \sum_{h=0}^{N-j} \bar{\varphi}_{h,j}(t)\varphi_{h}(\tau) \right] \varphi_{m-j}(t) \right] dt \]  

(2.280)

Due to \( \mathcal{P} = f_{aa}(t) dt \), \( f_{aa}(t) \) is found as

\[ f_{aa}(t) = \frac{\sum_{j=0}^{m} \dot{\Gamma}_{j}(t) \left[ \sum_{h=0}^{N-j} \bar{\varphi}_{h,j}(t)\varphi_{h}(\tau) \right] \varphi_{m-j}(t)}{\sum_{j=0}^{m} \left[ \sum_{h=0}^{N-j} \bar{\varphi}_{h,j}(t)\varphi_{h}(\tau) \right] \varphi_{m-j}(t)} \]  

(2.281)

Finally, by integrating \( f_{aa}(t) \), \( F_{aa}(t) \) can be introduced as

\[ F_{aa}(t) = \int_{0}^{t} f_{aa}(x) dx, \quad t \geq 0 \]  

(2.282)

The associated SEP can be also given as \( E_{aa} = 1 - F_{aa}(\tau) \). The integration in (2.282) cannot be solved analytically. However, \( F_{aa}(t) \) can be obtained by numerically
evaluating $(2.282)$ with Mathematica. This also includes the numerical derivation of $\dot{\Gamma}(t)$ that appears in $(2.281)$. 

Lemma 2.2. If the previous symbol is $b$, the cumulative distribution function for the delay of symbol $a$, i.e., $F_{ba}(t)$, is

$$F_{ba}(t) = \Phi_m(t)$$

and the associated SEP is $E_{ba} = 1 - F_{ba}(\tau)$.

Proof. For this case, there is no contributing molecule from the previous slot since the previous symbol is $b$ and $b \neq a$. Hence, the delay distribution can be expressed as $\Phi_k(t)$ which has been already derived in the proof of Lemma 2.1. 

By setting $N = 20$, $m = 12$, $d = 0.6\, \mu m$ and $D = 0.5\, \mu m^2/s$ in Fig. 2.31, $f_{aa}(t)$ is shown with regard to time for the different values of slot time $\tau$. As $\tau$ increases,
2.6 Communication Theories and Techniques for PMC Through Absorbers

The transmission of symbol $a$, an error arises if the delay experienced in the delivery of such symbol is higher than the slot time $\tau$. Therefore, in the case of $\tau = 0.1$, the probability of error is higher than the case of $\tau = 0.5$. Furthermore, the broader the curve of $f_{aa}(t)$ is, the lesser the error rate. This can be easily followed in Fig. 2.31. However, a longer slot time [or broader curve of $f_{aa}(t)$] also reduces the communication rate while providing a lower error rate.

In Fig. 2.32, $F_{aa}(t)$ is shown with respect to time according to the different values of the internode distance $d$. As $d$ decreases, the curve of $F_{aa}(t)$ becomes steeper. This is because the TN can deliver symbol $a$ more easily as it is closer to the RN. In other words, as the TN and RN are closer to each other, the propagation delay of the molecules decreases and this makes $F_{aa}(t)$ steeper as $d$ decreases. Hence, by combining the results in Fig. 2.31 and 2.32, it can be easily concluded that if the slot time is set to an extremely low value, the error rate becomes significantly high for the TN and RN that are relatively far from each other. In contrast, if the slot time is set to a significantly high value, the PMC performance reduces dramatically. Hence, $\tau$ should be selected in accordance with $d$.

In Fig. 2.33, $F_{ba}(t)$ is shown with time for the varying number of $N$. Here, the threshold $m$ used to decode symbol $a$ is set to $m = 10$ and $N$ is changed from $N = 15$ to $N = 30$. As observed in Fig. 2.33, the curve of $F_{ba}(t)$ becomes steeper as $N$ is increased. This also implies that the error rate and the delay can be decreased by properly selecting $N$ and $m$. Furthermore, the gap between the curves decreases as $N$ increases. For example, the gap between the curves for $N = 15$ and $N = 20$ is the maximum. This also reflects that the error is the highest for this case. Hence, the error rate can also be reduced by increasing $N$. However, $N$ can be viewed as a resource of PMC since the TN consumes an energy to synthesize and emit each molecule. Therefore, $N$ should be selected properly to minimize the resource consumption.

### 2.6.8 Binary Modulation Based on Molecular Arrays

All of the PMC schemes introduced above require exact time synchronization between the TN and RN. However, such a precise time synchronization may be beyond the state-of-the-art capabilities of very low-end nanomachines. Therefore, it is imperative for the realization of PMC systems to develop synchronization-free and practical PMC schemes. In this section, molecular array-based communication (MARCO) scheme is introduced, in which information messages are encoded by using the transmission order of the molecules as shown in Fig. 2.34 [7].

Let assume that two different molecules, called $a$ and $b$, are used to transmit information. The transmission order $a - b$ is used to transmit bit 0 and $b - a$ for bit 1. For example, suppose that the TN transmits 0 using the molecular order $a - b$ and the RN correctly receives this symbol as shown in Fig. 2.35. The correct reception probability of 0, i.e., $Pr(0|0)$, can be given by
**Fig. 2.33** \( F_{ba}(t) \) is shown with time for the different number of molecules, i.e., \( N \), which is emitted by the TN to transmit an information symbol.

**Fig. 2.34** Illustration of molecular order-based communication. Here, two distinct molecules, i.e., molecule type \( a \) and \( b \), are used to transmit information.

**Fig. 2.35** Transmission and correct reception of two molecules in order \( a - b \) which corresponds to the symbol 0.

\[
Pr(0|0) = Pr(t_b > t_a - t_e) \\
= 1 \times Pr(t_a < t_e) + I(t_e, \lambda) \times [1 - Pr(t_a < t_e)]
\]  
(2.284)
where \( t_a \) and \( t_b \) are the random time delays experienced by molecule \( a \) and \( b \), respectively. \( t_e \) is the inter-emission time of molecules (see Fig. 2.35). Molecules \( a \) and \( b \) are assumed to have the same diffusion coefficient. Then, \( t_a \) and \( t_b \) are assumed to have the same probability distribution as already given in (2.226). Hence, the transmission of symbol 0 with the order \( a - b \) is the same event with the transmission of symbol 1 using the order \( b - a \), which means \( Pr(0|0) = Pr(1|1) \). \( \lambda \) is a constant given by \( \lambda = d / \sqrt{D} \), where \( d \) is the distance between the TN and RN and \( D \) is the diffusion coefficient. Finally, \( I(t_e, \lambda) \) denotes the probability function and using the probability distribution of \( t_a \) and \( t_b \) in (2.226) and (2.227), respectively, it can be derived as

\[
I(t_e, \lambda) = \int_{t_e}^{\infty} \int_{t_a - t_e}^{\infty} f(t_a, t_b) dt_a dt_b
= \int_{t_e}^{\infty} \int_{t_a - t_e}^{\infty} f(t_a) f(t_b) dt_a dt_b
= \int_{t_e}^{\infty} f(t_a) \text{erf} \left( \frac{\lambda}{2\sqrt{t_a - t_e}} \right) dt_a
\]

(2.285)

where \( f(t_a, t_b) = f(t_a) f(t_b) \) since \( t_a \) and \( t_b \) are assumed to be independent. Using (2.226), \( Pr(t_a < t_e) \) in (2.284) can be computed as

\[
Pr(t_a < t_e) = \int_0^{t_e} f(t_a) dt_a
= \int_0^{t_e} f(t) dt
= \text{erfc} \left( \frac{\lambda}{2\sqrt{t_e}} \right)
\]

(2.286)

Substituting (2.285) and (2.286) into (2.284), \( Pr(0|0) \) becomes

\[
Pr(0|0) = \text{erfc} \left( \frac{\lambda}{2\sqrt{t_e}} \right) + \left[ 1 - \text{erfc} \left( \frac{\lambda}{2\sqrt{t_e}} \right) \right] \int_{t_e}^{\infty} f(t_a) \text{erf} \left( \frac{\lambda}{2\sqrt{t_a - t_e}} \right)
\]

(2.287)

\( Pr(0|0) \) is plotted in Fig. 2.36 as the inter-emission time \( t_e \) varies for different values of \( d \). While \( d \) decreases and \( t_e \) increases, \( Pr(0|0) \) increases. The results in Fig. 2.36 also reveal that \( Pr(0|0) \) becomes almost independent of \( t_e \) for sufficiently large \( d \). This is because \( t_e \) becomes irrelevant and any molecule may arrive first for the large values of \( d \).

Let us consider two consecutive binary symbols. In this case, it is possible for consecutive symbols to experience inter-symbol interference (ISI), and this may cause error in the channel. Let us assume that a transmitted symbol only interferes with either previously or next transmitted symbols. For example, if 0 is transmitted,
Fig. 2.36 $Pr(0|0)$ is shown with the varying values of the inter-emission time $t_e$ for the different distances $d$ between the TN and RN.

Fig. 2.37 Time diagram is shown for the transmission and correct reception of three consecutive symbols 000 which are transmitted by emitting $a-b, a-b, a-b$.

It may be interfered by the previous and the next symbols in the symbol triplets 000, 001, 101, and 100. If 1 is transmitted, it may be interfered by the previous and the next symbols in the symbol triplets 010, 011, 111, and 110.

Let us consider the transmission of symbol triplet 000 as shown in Fig. 2.37 and focus on the first 0. Let $y$ be the maximum of delay experienced by the molecules $a$ and $b$, i.e., $y = \max(t_a, t_b + t_e)$. Since $t_a$ and $t_e + t_b$ are independent, the cumulative distribution function of $y$, i.e., $F_y(t)$, can be given by

$$F_y(t) = F_{t_a}(t)F_{t_e+t_b}(t), \quad t \geq t_e \tag{2.288}$$

where $F_{t_e+t_b}(t) = F_{t_b}(t-t_e)$. $F_{t_a}(t)$ and $F_{t_b}(t)$ are the cumulative distribution functions given in (2.227), i.e.,
\[ F_{ta}(t) = F_{tb}(t) = F(t) = 1 - \text{erf} \left( \frac{d}{2\sqrt{D}t} \right) \]  

(2.289)

Then, \( F_y(t) \) in (2.288) becomes

\[ F_y(t) = F_{ta}(t)F_{te} + F_{tb}(t) 
= F_{ta}(t)F_{tb}(t-t_e) 
= \left[ 1 - \text{erf} \left( \frac{d}{2\sqrt{D}t} \right) \right] \left[ 1 - \text{erf} \left( \frac{d}{2\sqrt{D(t-t_e)}} \right) \right] \]  

(2.290)

The derivative of (2.288) also gives the probability density function of \( y \), i.e., \( f_y(t) \), which can be given as

\[ f_y(t) = f(t)F(t-t_e) + F(t)f(t-t_e), \quad t \geq t_e \]  

(2.291)

Let us consider the second 0 in the triplet 000. The delays of molecules \( a \) and \( b \) in the second 0 are represented by \( t'_a \) and \( t'_b \), respectively, as shown in Fig. 2.37. Using \( t'_a \) and \( t'_b \), let us define two other random variables \( z' \) and \( y' \) as \( z' = \min(t'_a + T, t'_b + t_e + T) \) and \( y' = \max(t'_a + T, t'_b + t_e + T) \), where \( T \) is the inter-symbol time (see Fig. 2.37). The cumulative distribution function of \( z' \), i.e., \( F_{z'}(t) \), can be derived as

\[ F_{z'}(t) = F(t-T) + F(t-t_e-T) - F(t-T)F(t-t_e-T), \quad t \geq T \]  

(2.292)

The derivative of \( F_{z'}(t) \) yields the density function of \( z' \), i.e.,

\[ f_{z'}(t) = f(t-T) \left[ 1 - F(t-t_e-T) \right] + f(t-t_e-T) \left[ 1 - F(t-T) \right], \quad t \geq T \]  

(2.293)

Now, similar to the first and second 0, consider the third symbol 0. The molecules \( a \) and \( b \) used for the transmission of the third 0 are denoted as \( t''_a \) and \( t''_b \), respectively (see Fig. 2.37). Let \( z'' \) be also the random variable that characterizes the minimum of \( t''_a + 2T \) and \( t''_b + t_e + 2T \), i.e., \( z'' = \min(t''_a + 2T, t''_b + t_e + 2T) \). The density function of \( z'' \), i.e., \( f_{z''}(t) \), can be also derived by replacing \( T \) in \( f_{z'}(t) \) given in (2.293) with \( 2T \), i.e.,

\[ f_{z''}(t) = f(t-2T) \left[ 1 - F(t-t_e-2T) \right] + f(t-t_e-2T) \left[ 1 - F(t-2T) \right], \quad t \geq 2T \]  

(2.294)

Consequently, by using the defined variables, the probability of ISI, i.e., \( P_{ISI} \), can be given as
where $P_{\text{NoISI}}$ is the probability that a transmitted symbol does not interfere with any other symbol and $Pr(y' < \alpha''|z' > y)$ can be derived as

$$Pr(y' < \alpha''|z' > y) = Pr(t_a' + T < \alpha''|t_a' + T > y)Pr(t_a' + T > t_b' + t_e + T) +$$

$$+ Pr(t_b' + t_e + T < \alpha''|t_a' + T > y) \times$$

$$\times Pr(t_b' + t_e + T > t_a' + T)$$  (2.296)

In (2.296), the two possible cases can be defined, i.e., either $y' = t_a' + T$ and $z' = t_b' + t_e + T$ or $y' = t_b' + t_e + T$ and $z' = t_a' + T$. Due to the independence of $t_a'$ and $t_b'$, (2.296) can be rewritten as

$$Pr(y' < \alpha''|z' > y) = Pr(t_a' < \alpha'' - T)Pr(t_a' > t_b' + t_e) +$$

$$+ Pr(t_b' < \alpha'' - t_e - T)Pr(t_a' < t_b' + t_e)$$  (2.297)

where $Pr(t_a' < t_b' + t_e) = Pr(0|0)$ and $Pr(t_a' > t_b' + t_e) = 1 - Pr(0|0)$. Note that $Pr(0|0)$ has been derived in (2.287). Hence, (2.297) becomes

$$Pr(y' < \alpha''|z' > y) = Pr(t_a' < \alpha'' - T) \left[ 1 - Pr(0|0) \right] +$$

$$+ Pr(t_b' < \alpha'' - t_e - T)Pr(0|0)$$  (2.298)

$Pr(t_a' < \alpha'' - T)$ in (2.298) can be modified as

$$Pr(t_a' < \alpha'' - T) = Pr(t_a' - \alpha'' < -T)$$  (2.299)

Let $r = -\alpha''$ and using $f_{\alpha''}(t)$ in (2.294), the density function of $r$, i.e., $f_r(t)$, is

$$f_r(t) = f(-t - 2T) [1 - F(-t - t_e - 2T)] +$$

$$+ f(-t - t_e - 2T) [1 - F(-t - 2T)], \quad t \leq -2T$$  (2.300)

Since $t_a$ and $r$ are independent, the density function for $t_a + r$, i.e., $f_{t_a+r}(t)$, can be obtained by the following convolution operation:

$$f_{t_a+r}(t) = \int_\bar{u}^\infty f(u)f_r(t - u)du$$  (2.301)

where $\bar{u} = \max(0, t + 2T)$. Using $f_{t_a+r}(t)$, $Pr(t_a' < \alpha'' - T)$ can be computed as

$$Pr(t_a' < \alpha'' - T) = Pr(t_a' + r < -T)$$
2.6 Communication Theories and Techniques for PMC Through Absorbers

\[ F_{t_a+r}(-T) = \int_{-\infty}^{-T} f_{t_a+r}(t)dt \]  

(2.302)

Furthermore,

\[ Pr(t'_a < z'' - t_e - T) = \int_{-\infty}^{-t_e-T} f_{t_a+r}(t)dt \]  

(2.303)

can be written. Then, \( Pr(y' < z''|z' > y) \) can be written as

\[ Pr(y' < z''|z' > y) = q(T)(1 - Pr(0|0)) + q(t_e + T)Pr(0|0) \]  

(2.304)

where \( q(x) \) is defined as

\[ q(x) = \int_{-\infty}^{-x} f_{t_a+r}(t)dt \]  

(2.305)

By substituting (2.304) into (2.295), \( P_{ISI} \) can be expressed as

\[ P_{ISI} = 1 - \left[ q(T)\left[1 - Pr(0|0)\right] + q(t_e + T)Pr(0|0)\right]Pr(z' > y) \]  

(2.306)

Let \( s = -y \). Then, \( Pr(z' < y) \) in the \( P_{ISI} \) expression can be expressed as

\[ Pr(z' < y) = Pr(z' + (-y) < 0) = Pr(z' + s < 0) \]  

(2.307)

Using \( f_y(t) \) in (2.291), the density function of \( s \) can be derived as

\[ f_s(t) = f_y(-t) = f(-t)F(-t - t_e) + F(-t)f(-t - t_e), \quad t \leq -t_e. \]  

(2.308)

Since \( z' \) and \( s \) are two independent random variables, the density function \( f_{z'+s}(t) \) can be obtained by

\[ f_{z'+s}(t) = \int_{-\infty}^{\infty} f_{z'}(u)f_s(t-u)du \]

\[ = \int_{-\infty}^{T} f_{z'}(u)f_s(t-u)du \]

\[ = \int_{-t_e}^{\infty} f_{z'}(u)f_s(t-u)du \]  

(2.309)

where \( \sigma = \max(t + t_e, T) \) and \( f_{z'}(t) \) has been already derived in (2.293). Then, \( Pr(z' < y) \) can be written as as
\[ Pr(z' < y) = Pr(z' + s < 0) = \int_{-\infty}^{0} f_{z'+s}(t)dt \] (2.310)

and thus, \( Pr(z' > y) \) is

\[ Pr(z' > y) = 1 - Pr(z' < y) = 1 - \tilde{p} \] (2.311)

where \( \tilde{p} \) is defined as

\[ \tilde{p} = Pr(z' < y) = \int_{-\infty}^{0} f_{z'+s}(t)dt \] (2.312)

Finally, by substituting \( Pr(z' > y) = 1 - \tilde{p} \) into (2.306), \( P_{ISI} \) in (2.306) can be given as

\[ P_{ISI} = 1 - \left[ q(T) \left[ 1 - Pr(0|0) \right] + q(t_e + T)Pr(0|0) \right] (1 - \tilde{p}) \] (2.313)

Substituting \( Pr(0|0) \), \( q(t) \), \( q(t_e + T) \), and \( \tilde{p} \) into (2.313), \( P_{ISI} \) can be also rewritten as

\[ P_{ISI} = 1 - \left[ \int_{-\infty}^{-T} \int_{-\infty}^{0} f(u)f_r(t-u)dudt \times \right. \]
\[ \left. \times \left[ 1 - \left( \text{erfc} \left( \frac{\lambda}{2\sqrt{t_e}} \right) + \text{erf} \left( \frac{\lambda}{2\sqrt{t_e}} \right) \int_{t_e}^{\infty} f(t_a)\text{erf} \left( \frac{\lambda}{2\sqrt{t_a-t_e}} \right) \right) \right] + \right. \]
\[ \left. + \left[ \int_{-\infty}^{-(t_e+T)} \int_{t_e}^{\infty} f(u)f_r(t-u)dudt \right] \times \right. \]
\[ \left. \times \left[ \text{erfc} \left( \frac{\lambda}{2\sqrt{t_e}} \right) + \text{erf} \left( \frac{\lambda}{2\sqrt{t_e}} \right) \int_{t_e}^{\infty} f(t_a)\text{erf} \left( \frac{\lambda}{2\sqrt{t_a-t_e}} \right) \right] \right) \times \]
\[ \left. \times \left[ 1 - \int_{-\infty}^{0} \int_{t_e}^{\infty} f_{z'}(u)f_s(t-u)dudt \right] \right) \] (2.314)

where \( f_{z'}(t) \), \( f_r(t) \), and \( f_s(t) \) are given in (2.293), (2.301), and (2.308), respectively. Furthermore, \( \pi \) and \( \sigma \) are given as \( \pi = \max(0, t+2T) \) and \( \sigma = \max(t+t_e, T) \).

In Fig. 2.38, \( P_{ISI} \) is plotted with the changing values of inter-emission time \( t_e \) and inter-symbol time \( T \). While the inter-symbol time increases, \( P_{ISI} \) decreases. As the difference between \( t_e \) and \( T \) becomes too small, \( P_{ISI} \) starts to increase. When the difference between \( T \) and \( t_e \) decreases below some critical values, \( P_{ISI} \) cannot be further reduced by increasing \( t_e \) and it starts to increase with \( t_e \).
In addition to $P_{ISI}$, the probability of error, i.e., $P_e$, can be formulated as

$$P_e = 1 - P_{NoISI(0|0)} Pr(0|0)$$

where $P_{NoISI(0|0)}$ is the probability that a symbol does not interfere given that it is correctly transmitted and it can be derived as

$$P_{NoISI(0|0)} = Pr\left( (z' > y) \cap (y' < z'') \mid (0|0) \right)$$

$$= Pr\left( y' < z'' \mid z' > y, (0|0) \right) Pr\left( z' > y \mid (0|0) \right)$$

(2.316)

where $Pr\left( y' < z'' \mid z' > y, (0|0) \right)$ can be given by

$$Pr\left( y' < z'' \mid z' > y, (0|0) \right) = Pr\left( t'_b + T < z'' \mid t'_a + T > y \right)$$

$$= Pr\left( t'_b < z'' - t_e - T \right)$$

(2.317)

$Pr(t'_b < z'' - t_e - T) = q(t_e + T)$ has been already derived [see (2.303) and (2.305)].

$Pr(z' > y \mid (0|0))$ in (2.316) can be also derived as

$$Pr\left( z' > y \mid (0|0) \right) = Pr\left( t'_a + T > y \right) = Pr\left( t'_a - y > -T \right)$$

(2.318)

Let us define another random variable $s$ as $s = -y$ and rewrite (2.318) as

$$Pr\left( z' > y \mid (0|0) \right) = Pr\left( t'_a + (-y) > -T \right) = Pr\left( t'_a + s > -T \right)$$

(2.319)

$f_s(t)$ has been already given in (2.308). $t'_a$ and $s$ are independent. Then, the density function of $t'_a + s$, i.e., $f_{t'_a+s}(t)$, is found as

$$f_{t'_a+s}(t) = \int_{-\infty}^{+\infty} f(u) f_s(t-u) du$$
\[ \int_{0}^{+\infty} f(u)f_s(t-u)du = \int_{\tilde{h}}^{+\infty} f(u)f_s(t-u)du \]  
\[ (2.320) \]

where \( \tilde{h} = \max(0, t + t_e) \). \( t_a \) and \( t'_a \) are the same delay variable in statistical sense and thus \( f_{t_a+s}(t) = f'_{t'_a+s}(t) \). Hence, \( Pr(z' > y|00) \) in (2.316) can be given as

\[ Pr(z' > y|00) = Pr(t'_{a} + s > -T) \]

\[ = 1 - F_{t_{a}+s}(-T) \]

\[ = 1 - \int_{-\infty}^{-T} f_{t_{a}+s}(t)dt \]

\[ = 1 - \bar{q}(T) \]  
\[ (2.321) \]

where \( \bar{q}(x) \) is a function defined as

\[ \bar{q}(x) = \int_{-\infty}^{-x} f_{t_{a}+s}(t)dt \]  
\[ (2.322) \]

By substituting (2.317) and (2.321) into (2.316), \( P_{NoISI|00} \) can be written as

\[ P_{NoISI|00} = Pr(y' < z''|z' > y, (0|0)) Pr(z' > y|00) \]

\[ = q(t_e + T)(1 - \bar{q}(T)) \]  
\[ (2.323) \]

Finally, using \( P_{NoISI|00} \), the error probability \( P_e \) in (2.315) can be written as

\[ P_e = 1 - P_{NoISI|00} Pr(0|0) \]

\[ = 1 - q(t_e + T)(1 - \bar{q}(T)) Pr(0|0) \]  
\[ (2.324) \]

where \( q(\cdot), \bar{q}(\cdot), \) and \( Pr(0|0) \) have been already introduced in (2.305), (2.322), and (2.287), respectively.

In Fig. 2.39, \( P_e \) is shown with varying values of \( t_e \) for the different values of \( T \). \( P_e \) and \( P_{ISI} \) follow almost the same characteristics. This is because \( P_e \) is directly a function of \( P_{ISI} \). However, the values of \( P_e \) are slightly higher than \( P_{ISI} \) (see Fig. 2.38 and 2.39). This increase stems from the fact that in some case there may be no ISI error while the symbol cannot be correctly received due to out of order of a single symbol with the probability \( (1 - Pr(0|0)) \).

Using \( P_e \), communication rate in the MARCO channel in bits per transmission, i.e., \( C \), can be characterized by \( C = (1 - P_e) \). Hence, by substituting \( P_e \), the communication rate, i.e., \( C = (1 - P_e) \), can be given by

\[ C = q(t_e + T)(1 - \bar{q}(T)) Pr(0|0) \]  
\[ (2.325) \]
Before ending this section, it is important to notice that further binary molecular communication schemes which are similar to ones introduced in this section can be found in [3, 29, 31, 34, 35].

References

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