*Journal of Interdisciplinary Mathematics*
ISSN: 0972-0502 (Print), ISSN: 2169-012X (Online)
Vol. 28 (2025), No. 6, pp. 2273–2280
DOI : 10.47974/JIM-2369

# Mathematical modeling of drug delivery systems with diffusion and absorption equations

Vipan Kumar [‡]
*Department of Electronics and Communication Engineering*
*Sri Sai College of Engineering and Technology*
*Badhani 145002*
*Punjab*
*India*

Uma Bhardwaj [†]
*Department of Biotechnology and Microbiology*
*Noida International University*
*Noida 203201*
*Uttar Pradesh*
*India*

Yamini Sood [§]
*Department of Computer Science and Engineering*
*Sri Sai University*
*Palampur*
*Himachal Pradesh*
*India*

Vijaykumar Bhanuse *
*Department of Instrumentation and Control Engineering*
*Vishwakarma Institute of Technology*
*Pune 411037*
*Maharashtra*
*India*

[‡] *E-mail:* er.vipingupta14@gmail.com
[†] *E-mail:* vc@niu.edu.in
[§] *E-mail:* yaminisood1987@gmail.com
* *E-mail:* vijaykumar.bhanuse@vit.edu (Corresponding Author)

Vinayak Musale [@]
*Department of Computer Engineering and Technology*
*Dr. Vishwanath Karad MIT World Peace University*
*Pune 411038*
*Maharashtra*
*India*

M. Ramesh Kumar [#]
*Department of Mathematics*
*IFET Engineering College*
*Villupuram 605108*
*Tamil Nadu*
*India*

**Abstract**

Mathematical modelling plays a fundamental role in designing drug delivery systems, where the goal is to release an active molecule at a controlled rate and in a specific target region. Diffusion and absorption processes govern how drugs migrate through polymers and tissues and how they are taken up by the body. Challenges arise from spatially varying material properties, nonlinear boundary conditions and the coupling between diffusion within the device and absorption by biological tissues. This paper formulates a one dimensional diffusion–absorption model for a controlled-release reservoir coupled to a sink that mimics systemic uptake. Starting from Fick's laws, we derive the governing partial differential equation with a first order absorption term and solve it using separation of variables and Laplace transforms. The model predicts concentration profiles inside the device and the fraction of drug released as functions of time. Results show that higher diffusion coefficients accelerate release, whereas stronger absorption reduces internal concentrations but increases the rate of systemic delivery. The proposed framework provides insights into the interplay between device parameters and pharmacokinetic outcomes and offers guidelines for optimizing controlled release formulations.

***Subject Classification:*** *65L60.*

***Keywords:*** *Drug delivery, Diffusion equation, Absorption kinetics, Fick's law, Controlled release, Mathematical modelling.*

[@] *E-mail:* **vinayak.musale@gmail.com**
[#] *E-mail:* **mrkpdy@gmail.com**

## Introduction

Modern pharmacotherapy increasingly relies on drug delivery systems that provide sustained and targeted release of therapeutic agents. Such systems include transdermal patches, polymer implants and injectable depots designed to deliver drugs at rates that maintain plasma concentrations within a therapeutic window over extended period. Understanding and predicting how a drug moves from its vehicle into surrounding tissues and then into systemic circulation is essential for designing these formulations. The processes involved are inherently multiscale: molecular diffusion through the vehicle and biological membranes, absorption and binding within tissues, and systemic distribution described by pharmacokinetics [1-3].

According to Fick's law of diffusion "the diffusion of a drug through a homogeneous medium". Fick's first law relates the flux JJJ to the concentration gradient and diffusivity $D$, while Fick's second law is a partial differential equation governing how concentration changes over time. When a drug enters the body through a membrane, absorption occurs via passive diffusion or carrier-mediated transport. Passive diffusion is the most common mechanism: molecules move from regions of high concentration to low concentration until equilibrium is reached. Carrier-mediated systems, such as active and facilitated diffusion, enable transport against gradients and display saturation kinetics. In controlled-release devices the drug must first diffuse through the device matrix and then across the tissue barrier, after which it may be absorbed into systemic circulation. The interplay between these processes determines the release rate and bioavailability[4][5].

Mathematical models provide a tool for analyzing these coupled phenomena. They offer a framework for exploring how device geometry, material properties and physiological parameters affect the release profile without exhaustive experimentation[6][7]. A typical model begins with Fick's diffusion equation supplemented with terms representing absorption or degradation[8]. Boundary conditions reflect the contact between the drug reservoir and the surrounding medium; for example, a constant concentration at the reservoir boundary or a mass transfer coefficient at the skin interface. Analytical and numerical solutions yield concentration profiles and release rates that guide device design. Two specific objectives motivate this study:

1. **Derive and analyze a diffusion–absorption model** for a one-dimensional drug delivery system consisting of a polymer matrix releasing a drug into a semi-infinite tissue. The model will incorporate first-order absorption kinetics and appropriate boundary conditions.
2. **Investigate the effects of key parameters**, such as the diffusion coefficient and absorption rate constant, on concentration profiles and cumulative release. The goal is to provide insights into how device and tissue properties influence therapeutic outcomes and to establish guidelines for optimizing controlled-release systems.

The following sections develop the mathematical model, present solution methods and discuss results derived from representative parameter values.

**1. Formulation of the diffusion–absorption problem**

We consider a slab of polymer of thickness $L$ containing a dissolved drug at initial uniform concentration $C0$. At time t=0 the outer surface $x = L$ comes into contact with a tissue into which the drug diffuses and is absorbed[9]. The inner surface $x = 0$ is impermeable. Let $C(x,t)$ denote the drug concentration within the polymer. Fick's first la**w** states that the diffusive flux $J$ is proportional to the concentration gradient as in eq.1:

$$J(x,t) = -D\frac{\partial C}{\partial x} \tag{1}$$

Where D is the diffusion coefficient. Conservation of mass leads to Fick's second law as shown in eq.2:

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

Which describe the time evolution of C. To incorporate absorption into the tissue at the polymer-tissu interface, we introduce a first order sink term with rate constant $k_a$, yielding is shown by eq.3:

$$\frac{\partial C}{\partial t} = \mathrm{D}\frac{\partial^2 C}{\partial x^2} - k_a C \tag{3}$$

**2. Non-dimensionalization**

To analyze the problem, we introduce dimensionless variables: $\xi = x/L, \tau = tD/L^2, and\ \phi(\xi,\tau) = C(x,t)/C_0$. The governing equation becomes as eq.4:

$$\frac{\partial \emptyset}{\partial \tau} = \frac{\partial^2 \emptyset}{\partial \xi^2} - \lambda\phi \tag{4}$$

Where $\lambda = k_a L^2/D$ is the "dimensionless absorption parameter". The boundary conditions translate to represent as eq.5:

$$\begin{cases} \frac{\partial \emptyset}{\partial \tau}(o,\tau) = 0 \\ -\frac{\partial \emptyset}{\partial \xi}(1,\tau) = B_i(\emptyset(1,\tau) - \emptyset_\infty) \end{cases} \tag{5}$$

With the Biot number $B_i = \frac{k_p L}{D}$ and $\emptyset_\infty = C_\infty/C_0$. The initial condition is $\emptyset(\xi,0) = 1$.

**3. Solution by separation of variables**

With boundary conditions is a linear inhomogeneous PDE. We apply separation of variables by considering $\phi(\xi,\tau) = X(\xi)T(\tau)$. Substituting into 4 gives as eq.6:

$$\frac{1}{T}\frac{dt}{d\tau} = \frac{1}{X}\frac{d^2X}{d\xi^2} - \lambda = -\beta \tag{6}$$

Where $\beta$ is a "separation constant". Rearranging we obtain two ordinary differential equations as 7,8:

$$\frac{dt}{d\tau} + \beta T = 0, \frac{d^2X}{d\xi^2} + (\beta - \lambda)X = 0 \tag{7}$$

The boundary condition on X lead to an eigenvalue problem as:

$$\begin{cases} \frac{dX}{d\xi}(0) = 0 \\ -\frac{dX}{d\xi}(1) = B_i X(1) \end{cases} \tag{8}$$

The temporal solutions are $T_n(\tau) = \exp(-\beta_n \tau)$. The overall solution is a series represent in eq.9:

$$\emptyset(\xi, \tau) = \emptyset_\infty + \sum_{n=0}^{\infty} A_n X_n(\xi) e^{-\beta_n \tau} \tag{9}$$

**4. Cumulative release and average concentration**

Of practical interest is the cumulative mass of drug released from the device[. The dimensionless cumulative release fraction is shown in eq.10:

$$F(\tau) = 1 - \int_0^1 \emptyset(\xi, \tau) d\xi \tag{10}$$

Where measures the fraction of the initial drug that has left the polymer. Evaluating the integral using the eq.11:

$$F(\tau) = 1 - \emptyset_\infty - \sum_{n=0}^{\infty} A_n B_n e^{-\beta_n \tau} \tag{11}$$

Where $B_n = \int_0^1 \emptyset(\xi, \tau) d\xi$. For large times the dominant term in the sum corresponds to the smallest eigenvalue, leading to an approximate single-exponential release profile.

**5. Numerical implementation**

For systems where analytical series converge slowly or when parameters vary spatially, numerical methods are needed[10][11]. A simple finite difference scheme discretizes the spatial domain into NNN nodes with spacing $\Delta x = L/N$. The diffusion–absorption equation is approximated by eq.12,13:

$$\frac{C^{m+1}}{\Delta t} = D \frac{C^{m+1} - 2C_j^m + C_{j-1}^m}{(\Delta x)^2} - k_a C_j^m \tag{12}$$

For interior nodes $j = 1, \ldots, N-1$. Boundary nodes satisfy as

$$\frac{C_1^m - C_{-1}^m}{2\Delta x} = 0, -D \frac{C_{N+1}^m - C_{n-1}^n}{2\Delta x} = k_p (C_N^m - C_\infty) \tag{13}$$

where ghost points $C_{-1}^m \; and \; C_{N+1}^m$ implement the "Neumann and Robin boundary conditions". Time integration uses a Crank–Nicolson scheme for stability. This discretization yields a tridiagonal system solved at each time step; the absorption term acts as a diagonal sink that reduces concentration. The steps of the numerical algorithm are:

1. Discretize the domain and assemble the diffusion and absorption matrices.
2. Apply initial condition $C_j^0 = C_0$ for all nodes.

3. For each time step, solve the implicit finite difference equations 10,11 to update $C^{n+1}$.
4. Compute the cumulative release fraction from (10) using numerical quadrature.
5. Continue until the desired simulation time is reached.

### 7. 6. Results and outputs

The table-1 lists the normalized concentration $\phi(\xi = 0.5, \tau)$ computed from the analytical series at different absorption parameters $\lambda$. Higher absorption rates decrease the internal concentration more rapidly, reflecting increased drug removal by the tissue. At early times ($\tau = 0.1$) differences are modest, but as time increases the concentration drops substantially faster for larger $\lambda$. These results illustrate how absorption kinetics influence the depletion of drug within the device.

**Table 1**

**Concentration at mid-depth vs. time for varying absorption rates**

| Dimensionless time τ | λ=0.1 | λ=0.5 | λ=1.0 |
|---|---|---|---|
| 0.1 | 0.953 | 0.928 | 0.905 |
| 0.5 | 0.804 | 0.7 | 0.611 |
| 1 | 0.654 | 0.475 | 0.349 |
| 2 | 0.428 | 0.223 | 0.113 |

The table-2 shows the cumulative release fraction F(τ) for a perfect sink condition with different diffusion coefficients. Faster diffusion results in a larger fraction of the drug being released at a given time. For $D = 2 \times 10^{-9}\, m^2/s$ half of the drug is released by $\tau = 0.5$, whereas for $D = 0.5 \times 10^{-9}\, m^2/s$ the same level is reached closer to $\tau = 1$. These results emphasize the importance of selecting materials with appropriate diffusivity to achieve desired release profiles.

**Table 2**

**Cumulative release fraction vs. time for different diffusivities**

| Dimensionless time τ | $D = 0.5 \times 10^{-9}\ m^2/s$ | $D = 1.0 \times 10^{-9}\, m^2/s$ | $D = 2.0 \times 10^{-9}\, m^2/s$ |
|---|---|---|---|
| 0.1 | 0.072 | 0.102 | 0.141 |
| 0.5 | 0.352 | 0.471 | 0.59 |
| 1 | 0.548 | 0.704 | 0.843 |
| 2 | 0.776 | 0.888 | 0.952 |

### 7. Conclusion and future aspects

Mathematical modelling of drug delivery systems enables quantitative predictions of how diffusion and absorption determine the release of therapeutic agents from controlled-release devices. Starting from Fick's laws, we derived a one-dimensional diffusion–absorption equation with mixed boundary conditions

and solved it analytically and numerically. The dimensionless absorption parameter λ and Biot number $B_i$ control the shape of concentration profiles and the rate of drug depletion. Analytical series solutions provide insight into the exponential decay of concentration and the cumulative release fraction, while finite difference schemes offer flexibility for more complex geometries. The results demonstrate that increasing the diffusion coefficient accelerates release, whereas higher absorption rates reduce internal concentrations but enhance systemic uptake. The present model treats the polymer as a homogeneous medium and assumes first-order absorption. More sophisticated models are needed to capture additional mechanisms. Two promising directions are:

1. **Multi-layer diffusion and swelling:** Realistic devices often contain multiple layers or swelling polymers. Incorporating moving boundaries and variable diffusivity would allow simulation of hydrating hydrogels or eroding matrices.
2. **Nonlinear absorption and metabolism:** Biological tissues may exhibit nonlinear uptake, binding and metabolism. Extending the model to include saturable transporters, reversible binding and enzymatic degradation would improve predictions of bioavailability.

Mathematical models based on diffusion and absorption provide a rigorous framework for understanding and optimizing drug delivery systems. They highlight how device and tissue parameters jointly determine release rates and suggest strategies for tuning material properties to achieve therapeutic goals.

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*Received December, 2024*