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Original Article

AI-Driven Molecular Communication for Targeted Drug Delivery with Adaptive Release Optimization

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Abstract *- Molecular Communication has emerged as a prominent area of research, particularly for drug-based medical therapies. Nanomachines are utilized to inject drugs (such as anti-inflammatory molecules) into the human body, targeting infected cells through communication technologies. Nevertheless, creating an effective Targeted Drug Delivery (TDD) system that minimizes drug wastage remains a significant challenge. Previous research has tackled various issues, including improper drug delivery and low success rates. These challenges have inspired us to set the goal of accurately delivering drugs to the intended location using molecular Communication in TDD. Furthermore, we propose an AI-enhanced TDD system aimed at achieving improved therapeutic outcomes for a range of conditions, including cancer and heart disease. This research also addresses the problems of high side effects, improper path selection, and inefficient drug delivery. The main objective of this research is to design an advanced targeted drug delivery using molecular Communication. So, we employ Artificial Intelligence (AI) technology for Targeted Drug Delivery with an adaptive Drug Release Rate optimization method (AI-TDD) to overcome the existing issues. We execute a Double Deep Q Network (DDQN)- based adaptive Drug Release method to minimize drug wastage. This method uses biomarker concentrations and timely signal provisioning from external devices and entities. This work's simulation is performed using Python-based simulations with fine-tuned system and simulation configurations. Our work's performance assessment is carried out using four major metrics: Delivery Error Analysis, RMSE Analysis, Drug Release Rate Analysis, and Drug Reception Rate Analysis, which shows that our proposed AI-TDD model outperforms the existing model.*

Keywords *- Molecular Communication, Targeted Drug Delivery, Adaptive Drug Release Rate, Artificial Intelligence, Nanomachines.*

1. Introduction

Molecular Communication is a biometric system that uses an aqueous environment to communicate with bio-machines [1]. Molecular Communication is an emerging field that explores the exchange of information using chemical molecules, mimicking natural biological communication processes to enable Communication between nano-scale entities in environments where traditional electromagnetic Communication is impractical. Molecular Communication serves as a biometric system that allows bio-nanomachines to communicate through an aqueous medium [2]. Recent advancements in Molecular Communication (MC) discuss biological, chemical, and physical processes, modulation techniques, and communication engineering aspects, while highlighting the need for interdisciplinary work and future research directions in engineering reliable MC systems [3]. Molecular Communication is a platform for transmitting text messages using chemical signals, demonstrating the feasibility of molecular Communication at macroscales. It emphasizes simplicity, cost-effectiveness, and motivates future research on realistic modeling and analysis of these systems [4]. Molecular communications applications in medicine, focusing on disease detection, treatment, immune System triggering, tissue engineering, and nanosurgery, targeted drug delivery while addressing challenges and future perspectives for implementing these advanced, minimally invasive, and biocompatible healthcare solutions [5]. Molecular Communication (MC) and Molecular Networks (MN) for Targeted Drug Delivery (TDD), discussing their potential to enhance drug localization, address challenges in clinical translation, and provide a framework for evaluating MC-based TDD systems and their implementation [6]. By delivering the medication to a specific location, the TDD lessens the likelihood of the medicine spreading throughout the body and avoids adverse consequences. The medications are contained in the nanomachines to lessen the harm to healthy cells [7]. The conventional medication system can spread the drug all over the body and harm healthy cells, which is the main cause of ineffective drug delivery.

Therefore, in order to build a smart medication delivery system that addresses the problems with conventional treatment approaches, the molecular communication system requires Artificial Intelligence (AI). The pharmacokinetic/pharmacodynamic models are enhanced by this kind of intelligent therapeutic Technology [8]. AI makes intelligent decisions to provide the right treatment for a patient, and it also manages the clinical data for future drug development. The AI addressed the time-consuming issues in traditional drug delivery systems, and it provides the drugs quickly and precisely [9].

Another key idea in TDD is drug route administration, which determines which medicine-topical, oral, or parental-is administered [10]. Clinicians choose the route based on patient convenience, which is partly influenced by pharmacokinetic characteristics [11]. Since an aqueous environment is used for Communication between the nanomachines and the targeted location, the best route for drug administration is crucial to boosting the success rate of drug delivery [12]. The best route is found by taking into account the location and direction of the targeted site and nanomachines. The nanomachines release the drug molecules by choosing the best route [13]. The nanomachines, which are typically implanted directly into the targeted region, are nanometers in size.

The medications are released from the nanomachines if they reach the intended location. To minimize drug waste and traffic, the release rate of drug molecules must be at its peak [14]. Static, then there is a set distance between the targeted spot and nanomachines [15, 16]. If the nanomachines are mobile, then the distance is adjusted dynamically; consequently, the drug molecule concentration is also dynamically modified. Therefore, to enhance the effectiveness of therapeutic drug delivery, it is essential to employ a dynamic and adaptive drug release mechanism that regulates the dosage in real time. Such an approach prevents excessive drug accumulation at the target site, minimizes potential side effects, conserves therapeutic resources, and significantly reduces treatment time. To address this drawback, we propose using AI Techniques to optimise both the drug delivery route and the adaptive drug release rate, thereby ensuring precise and personalized therapeutic outcomes**.**

2. Motivation & Objectives

The interaction between artificial materials and human body cells presents several problems for molecular Communication for tailored medication delivery systems.

Numerous issues, including improper medication administration and low success rates, have been addressed by current research, but no ideal answers have been offered. The following concerns were the subject of this study:

2.1.1. Poor Choice of Path

Few current studies are focused on optimum path selection for drug delivery; however, they examine only a restricted metric (i.e., direction), which is not adequate for optimal path selection that leads to a low success rate owing to the existence of barriers in the extracellular channel.

2.1.2. High Side Effects

Some current works do not optimize the timing and amount of medication delivery, which results in side effects from either an overdose or an underdosage of drug emission. Because the medications are absorbed by the healthy cells, ineffective target site localization also results in side effects.

2.1.3. Ineffective Drug Delivery

Ineffective drug delivery is caused by a lack of intelligence in the regulation of nanomachines and drug release rate. Furthermore, ineffective medication delivery is also caused by a lack of connection between transceivers. The effectiveness of therapeutic medications is decreased by the current work's consideration of static releasing rates for pharmaceuticals, which are not appropriate for all kinds of molecular compounds.

The above-described issues led us to suggest the goal of employing molecular Communication in TDD to swiftly and accurately deliver a medication to the intended location. Furthermore, the AI-based TDD is suggested to create a TDD system for improved treatment outcomes for a number of illnesses, including cancer, heart disease, and others. The issues of excessive side effects, poor route selection, and ineffective medication delivery are also covered in this study. The primary goal of this project is to use an adaptive drug release rate to manage the drug load and minimize drug waste, which also increases the effectiveness of therapeutic outcomes. We use the DDQN algorithm, which automatically learns the environment and takes an action that reduces toxicity and side effects, to perform an adaptive drug release rate, which is used to reduce drug waste and control drug load. The release rate is adaptively changed by considering biomarker concentration, location, and distance.

3. Literature Review

This section provides the literature review of the existing works in the molecular drug delivery system. Further, we also detail the existing literature work along with the corresponding Issue.

In order to address delivery-time errors caused by propagation delays, Tania et al. [17] propose a molecular communication-based simultaneous drug-delivery scheme using internal controller nanomachines to synchronize drug release from multiple nanomachines. This scheme improves energy efficiency and robustness, but random propagation delays cause delivery-time errors because drug-carrying nanomachines may not arrive simultaneously. Abd El-atty et

al [18] present a bio-cyber interface architecture coupling MC with IoBNT for intelligent TDD, emphasizing sustainable/energy-aware operation and end-to-end system blocks from sensing to drug release, but Closed-loop AI control is unspecified/unevaluated, as well as Security/privacy not co-designed with control.

Junejo et al. [19] suggested using a deep learning system to analyze diseases based on molecular Communication..In this study, a transmitter and receiver for a target medication delivery system employing molecular Communication were designed using a deep learning technique called Multilayer Perceptron Deep Neural Network Autoencoder. Biological signals are used to monitor the patient's health state, and patient health data is kept on the cloud. According to the simulation findings, the suggested work performed better in terms of accuracy and BER. This study designed a transceiver using a deep learning-based autoencoder method, which has a delayed convergence and requires a lot of training time, resulting in substantial transmission latency.

Sharifi et al. [20] This study proposed a touchable molecular communication system for targeted medication administration. Finding the best medication delivery strategies that minimize pharmacokinetic system uncertainty is the primary goal of this study. In order to incorporate the random concentration of tumour sites, a tumour immune communication model was suggested. A new controller for spreading the best medication delivery plan was presented in this study. While the blood vessel is in charge of drug transportation, the nanorobots transport the drug and inject it into the human body for signal transmission and reception. Islam et al. [21] To achieve high accuracy during sequential medication administration, this research presented a multidrug delivery approach. Controlling the drug's release timing is the primary goal of this study.

Here, a controller nanomachine implanted in the human body managed drug-carrying nanomachines. Three nanomachines-a controller, a releaser, and a monitor-are part of the suggested project. The controller then estimates the medication release time by calculating the difference between the first and second drug delivery times. Lastly, the difference between the present and real medication time interval was taken into account when estimating the inaccuracy. The experimental findings show that the suggested work performed better in terms of medication release intervals. Nanomachines were suggested in this work for the best possible medication delivery; nonetheless, large delivery time mistakes result from a lack of intelligence during drug administration. Monteiro et al. [22] A suggested deep learning approach for drug target interaction prediction was presented in this publication. The deep learning method used raw data and SMILES strings to determine the drug-protein interaction. Here, interaction prediction was done using a mix of a fully connected network technique and a convolutional neural network. Two parallel convolution methods were used by the suggested convolution neural network approach to extract the features from the data. Lastly, conventional machine learning techniques were used to compare and assess the suggested deep learning algorithms. The experimental findings demonstrate that, in comparison to conventional machine learning methods, the suggested work performed better. Due to the generation of undesired convolutional layers that increase prediction time, two parallel convolutional neural networks were proposed for target interaction prediction, which results in a significant communication delay..

Al-Zubi et al. [23] To forecast the spatiotemporal attention of anticancer medications in tumour microenvironments, our study put out a numerical and simulation model. This study used molecular Communication to develop a mathematical model for channel impulsive response with drug release rate. The drug's physicochemical characteristics were used to alter the release rate. Lastly, a stochastic simulation model was introduced for simulating drug interaction and transportation. The drug release rate was predicted using a MATLAB simulation tool. The outcomes demonstrated that the suggested approach performed better in terms of medication release rate in the tumour microenvironment. In this case, the drug release rate was altered by taking into account physicochemical characteristics, which were insufficient to identify the ideal release rate that influences the therapeutic outcomes due to ineffective drug delivery.

The targeted drug delivery models for cancer applications are estimated by Tang et al. in [24]. The many nano-system models for cancer recovery applications are examined in this research. Nanoemulsion, nanogel, exosome, hybrid NP, rHDL, dendrimer, micelle, and liposome are among the several encapsulation types. Any of the aforementioned methods is used to encapsulate the medications, which are subsequently injected into the human body and activated at the target (i.e., cancer cells).

In this case, targeted medication administration was carried out for the cancer application, but less precision was achieved when choosing the best route. A drug detection model with nanoparticle assistance for cancer applications was designed by Raj S. Khurana et al. [25]. For practically every portion of the human body, a number of approaches were examined. With or without a designated target, the nanoparticles functioned as therapeutic agents. Adopting medicine delivery based on nanoparticles makes it simple to identify malignant cells and release medications to overcome them without potentially harmful consequences. Notably, the adverse consequences of medication delivery based on nanoparticles must also be taken into account.

4. Problem Statement

Along with related issues and answers, the section addresses the main problem statements in this particular body of previous work.

El-Fatyany A. et al. [26] used the Internet of bio-NanoThings to propose a target medicine delivery system. The primary goal of this study was to develop an ideal model for enhancing the effects of medication delivery by employing an end-to-end system to target therapy at the target spot.

In contrast to the proposed technique, which uses two communication types-forward link and reverse link-the doctor initially transmitted the data to the transmitter via an access point. The issues mentioned in this method include

- In this case, forward and reverse link communication was used to increase the rate of medication delivery; nevertheless, it fails to take into account the best route from the source to the target location, resulting in a lower success rate.
- R2 is in charge of drug emission in this case, but the amount and timing of drug release are not regulated or optimized, which results in side effects from either an excessive or insufficient rate of drug release for the target cell.

A novel approach to drug release rate optimization for targeted drug delivery devices was presented by Zhao et al. [27]. Measuring the optimal medication release rate is the primary goal of this study. The intended site's closest position was where the nanomachine was immediately inserted. In this case, the targeted location served as a receiver and the nanomachine as a transmitter. The issues mentioned are

- In this case, location and distance were used to optimize the medicine delivery rate, which was insufficient. Furthermore, the continuous medication delivery rate predicted by this study is insufficient to provide therapeutic medicines.
- Drug delivery systems are less effective when there is a lack of communication tracking between the transmitter and the receiver.

4.1. Research Solution

The following are the difficulties raised in the specific existing studies stated above. The primary goal of this research is to improve the effectiveness of molecular Communication by minimizing medication waste. Using the DDQN algorithm based on dynamic distance, dynamic location, and biomarker concentration, the adaptive drug release is carried out. Finally, the error between drug delivery times is computed and updated as feedback to improve efficacy.

5. Methodology

Using Double Deep Q-Network (DDQN) for Targeted Drug Delivery (TDD), we can optimize the nanomachine's path planning in a dynamic blood environment, considering factors like obstacles (blood clots), blood flow, velocity, and target site location. Blood flow is highly dynamic and unpredictable. DDQN adapt to changing conditions without overestimating path values.

The nanomachines in the targeted site release the drug molecules by using the adaptive release rate method. Here, the drug release rate adaptively changes by considering biomarker concentration, dynamic location, and dynamic distance. The nanomachines are tracked by the clinician to update the current location and distance. The clinician sends the signal to the nanomachine for drug release time, load, and location. Here, an improved reinforcement learning algorithm, namely Double Deep Q Network (DDQN), is proposed for adaptive drug release, in which the DDQN automatically balances the exploration and exploitation for increasing the performance of adaptive drug release rate, which reduces drug wastage and controls drug load.

The proposed DDQN is based on a markov decision process composed of tuples representing the state, the action space, the transition, and the reward. Table 1 denotes the illustration of state, action, and rewards towards the real-time environment.

Table 1. Proposed DDQN parameters

DDQN Parameters	Description
Agent	The drug nanomachine.
State (st)	Representation/Features of Environment's position (x,y), velocity, and surrounding obstacle data(blood clot)
Action (ac)	Movement in discrete directions at any given time (left, right, forward, backwards). Performs adaptive drug release
Reward (rew)	Performance improvement and drug wastage reduction Positive reward for moving towards the target and drug release. Negative reward for collisions with obstacles (e.g., blood clots).
Next state ($st+1$)	The next state is updated based on the selection policy of the nodes

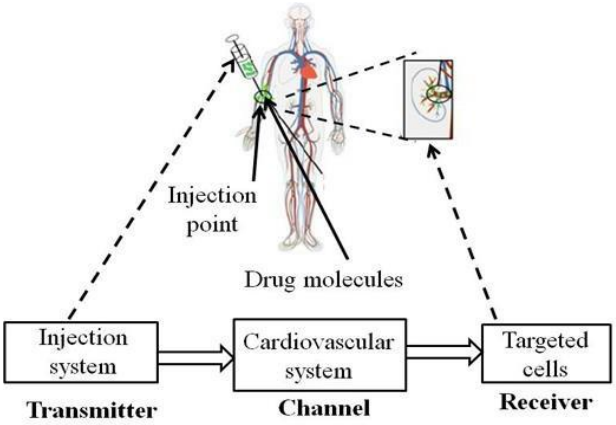

Fig. 1 Molecular Communication-Based Targeted Drug Delivery Model [28]

The proposed DDQN is introduced to increase the learning rate by learning in the offline environment. Clearly, during training, the exploitation and exploration rate can be controlled adaptively by mixing the training samples. In addition, performance improvement is achieved by introducing a greater Q-network in the proposed design. To overcome the Issue of improper interaction with the environment, we have introduced an ordered storage method to permanently store the interactions on the agents in the reply buffers. Only the amplified policy data can be stored in the buffer, whereas the lesser policy data cannot be stored; thus, the mixing control can be effectively achieved.

A molecular communication system in drug delivery consists of three primary components, as shown in Figure 1.

5.1. Transmitter (Drug Carrier)

The transmitter is responsible for releasing the drug molecules into the biological environment.

5.1.1. Channel

The channel is the medium through which drug molecules propagate from the transmitter to the target cells. The characteristics of the channel determine the effectiveness of drug transport. Key channels include:

- Bloodstream: The most common medium, where drug molecules diffuse through blood plasma and interact with cells.
- Extracellular Fluid (ECF): Drugs diffuse through interstitial fluid in tissues to reach target cells.

5.1.2. Receiver (Target Cells/Tissues)

The receiver is the site where the drug molecules bind and initiate a therapeutic effect.

Figure 2 below is the proposed DDQN-based drug release. The diagram given below represents a proposed Double Deep Q-Network (DDQN) Algorithm for adaptive drug release in a molecular communication-based targeted drug delivery system.

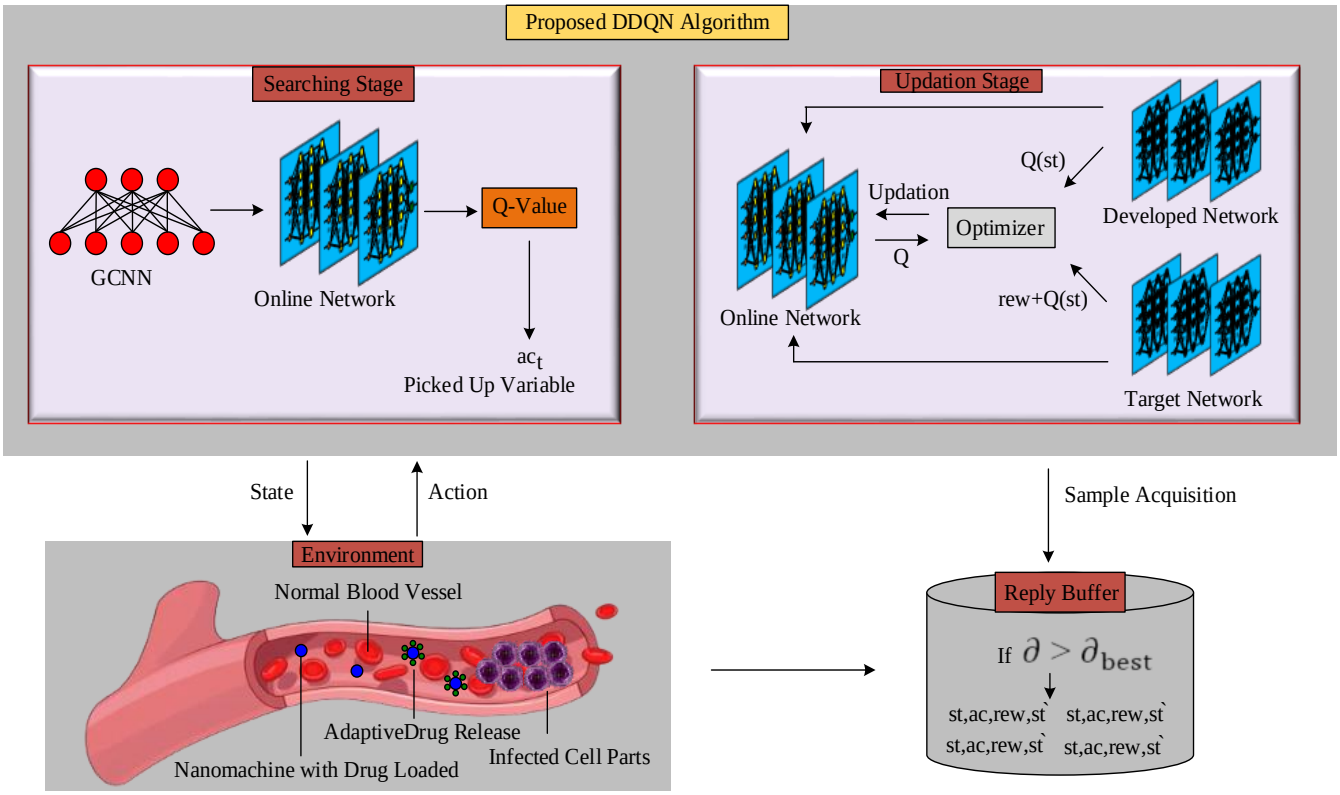

Fig. 2 DDQN algorithm-based adaptive drug release

Figure 2 consists of four sections, which can be elaborated as follows.

- Searching Stage: A Graph CNN (G-CNN) Processes the Environment, and The Online Network Selects the Best Action Based On Q-Values.
- Environment Interaction: A Nanomachine Releases Drugs in A Blood Vessel, Adapting to Infected Regions.
- Reply Buffer: Stores State-Action-Reward Data and Updates If a Better Reward Is Found.
- Updating Stage: The Online Network is Trained Using Stored Experiences, and The Target Network is Updated Periodically to Refine Drug Delivery Decision.

DDQN uses two networks to separate action selection from action evaluation:

- Online Network (Θ) - This primary network learns from experience, updates during training, and selects the best action.

$$b^* = argm \max Q(S', b', \theta^-) \quad (1)$$

b^* : The best possible action to take in the state s′
argm max: argument that maximizes Q-value.
$Q(s', b'; \theta)$: The estimated Q-value of taking action b' in state s', given parameter θ.

- Target Network (Θ-) – This is a delayed copy of the online network, updated periodically (not every step) and evaluates the action's Q-value.

$$Q(S', b^*, \theta^- \quad (2)$$

Q(s′,b∗; Θ-) is the Q-value function that estimates the expected future reward for taking the optimal action b^* in the next state s′.

θ^- Represents the parameters of the target network, which is a separate set of weights used for more stable learning.

b∗ is the optimal action selected using the online Q-network.

The target network is updated periodically to improve training stability and reduce the problem of moving target values.

The expression below is a crucial part of the target value calculation in DDQN updates:

$$y = r + \lambda Q(S', b^*, \theta^- \quad (3)$$

Where y is the target Q-value, r is the immediate reward, and λ is the discount factor.

5.1.3. DDQN Update Rule

Instead of directly taking the maximum Q-value for the next state, DDQN updates Q-values as:

$$Q(s, b) = r + \lambda \text{Qtarget}(\text{s}', \arg max\ \text{Qonline}(s', b')) \quad (4)$$

Q(s,b) is the Q-value function estimating the expected reward for taking action b in state s.
r is the immediate reward obtained after taking action b.
λ is the discount factor (typically between 0 and 1), which determines the importance of future rewards.
Q_{target} is the Q-value from the target network.

Arg max Q_{online}(s', b') selects the best action in the next state s′ using the online network.

Instead of directly using the target network to select and evaluate actions (as in DQN), Double Q-learning first selects the best action using the online network and then evaluates it using the target network. This helps reduce overestimation bias. Target, online, and developed networks are the three sub-networks that make up the larger Q-network that was introduced. The online network is used to choose the action, the target network serves as an action evaluator, and the generated network functions as a Q-network. Furthermore, Graph Convolutional Neural Networks (GCNNs) may be used to parameterize the suggested Q-network. GCNN involves two sub-phases: variables to constraints and constraints to variables. Below is a formulation of the suggested DDQN restrictions,

$$\mathcal{E}_j \leftarrow f_\mathcal{E}\left(\mathcal{E}_j, \sum_i^{(j,i)\in\mathcal{E}} \varphi_\mathcal{E}\left(\mathcal{E}_j, \omega_i, \Upsilon_{j,i}\right)\right) \quad (5)$$

$$\omega_j \leftarrow f_\omega\left(\omega_j, \sum_i^{(j,i)\in\mathcal{E}} \varphi_\omega\left(\mathcal{E}_j, \omega_i, \Upsilon_{j,i}\right)\right) \quad (6)$$

From the above equations (5) and (6), the ReLU activation function double-layer perceptron can be denoted as $f_\mathcal{E}$, f_ω, $\varphi_\mathcal{E}$, and φ_ω respectively. Furthermore, the overall loss function of the proposed DDQN can be formulated as,

$$\text{Loss}(\theta) = \mathbb{E}\left(\text{rew} + \text{ɤ} \max_{ac'} \mathbb{Q}^{t}(st', ac', \theta^{t}) - \mathbb{Q}(st, ac, \theta)\right) + \mathbb{E}\left(\mathbb{Q}^{dev}(st, ac, \theta^{dev}) - \mathbb{Q}(st, ac, \theta)\right) \quad (7)$$

From the above equation, the script t and dev represent the target and developed network, respectively. The pseudocode for the proposed DDQN-based drug release can be provided as given.

Pseudocode for DDQN-based adaptive drug release
Initialize: → Random Initialization of θ → Random Initialization of θ^t → Random Initialization of θ^{dev} Target network update frequency fre^t Policy evaluation frequency fre^{dev} Policy assessment threshold ∂_0

```
Cumulative reward policy during training ∂_best
For Steps T ∈ 1,2…., do
  Get trial action from policy behaviour ac~π^(ℚ^dev)
  Perform ac and perceive (st′, rew)
  Stock (st, ac, rew, st′) → Buff^Temp
  Get a mini-batch sample from Buff^Reply
  Compute Loss based on (12)
  Update θ using gradient descent
  If t mod ϒ^t = 0 then
    θ^t ← θ
  End If
  If t mod ϒ^dev = 0 then
    Calculate ∂ for policy training assessment
    If ∂ > ∂_best then
      θ^dev ← θ
    End If
    If ∂ > ∂_0 then
      Stock (st, ac, rew, st′) → Buff^Temp, Buff^Reply
      Overwrite the oldest policy
    End If
  End If
  dev ← dev′
End For
End
```

Ultimately, we assess the error in drug delivery time by analyzing both the fastest and slowest delivery times. The collected error rates are fed back into the DDQN, which helps to minimize the delivery time discrepancies. This approach enhances therapeutic drug efficacy and pharmacokinetics systems. Moreover, it mitigates side effects and toxicity associated with both excessive and insufficient medication dosages in targeted drug delivery systems. The cloud server retains all environmental data for ongoing patient health monitoring. This method streamlines targeted drug delivery by enhancing precision and minimizing waste. The system and simulation configurations are provided in Tables 2 and 3, respectively.

Table 2. System configurations

Software Settings	Processer	AMD Ryzen 7 5700U with Radeon Graphics 1.80 GHz
	Operating System	Windows 10
	Simulation Software	Python 3.10.11
Hardware Settings	Random Access Memory	6GB
	Hard Disk	1 TB

Table 3. Simulation parameter

Simulation Parameter	Description
No. of Nano machine nodes	5
No. of Receptors	25
Time step duration	200ns
Coefficient of diffusion	$1 \times 10^{-2}\mu m^2/\mu s\mu s$
Radius of space receptors	250nm
Time step for simulation	0.005s
Time interval for drug delivery	{1,10} Min
Molecules Released	6K,8K,10K,12K Molecules
Radius of a nanomachine	{5,7,9,11,13}μm

6. Results and Discussion

This section details the experimental results of the proposed work in both qualitative and quantitative manners. Further, this section also provides a comparative analysis of the proposed and existing works to enumerate the performance of the proposed work. The supplementary sections in the experimental results are explained as follows,

6.1. Comparative Analysis

This section summarizes the quantitative and qualitative study of the suggested AI-TDD model, as well as previous studies like Release rate Optimization for Targeted Drug Delivery (Optimized-TD) [27] and Internet of Bio-nano Things-based Targeted Drug Delivery (IoBT-TD) [26]. Delivery error, RMSE, medication release rate and drug reception rate are the assessment criteria used.

6.2. Implemented System

We built an AI "agent" that learns when and how much drug to release while moving through a noisy blood environment.

- It gets a high score ("reward") when the drug reaches the target site quickly and safely, using a minimal dose.
- It loses points for delays or off-target exposure.
- Each episode is one full simulated delivery attempt.
- Epsilon (ε) tells how often the agent still tries random actions (exploration). A smaller ε means it's mostly following what it has learned.

Figure 3 shows the output of the final episodes of DDQN training for targeted drug delivery. Each line lists the episode number, achieved reward, and epsilon value.

Rewards fluctuate but remain relatively high, indicating the agent has learned effective strategies. The steadily decreasing epsilon (from ~0.09 to ~0.08) reflects reduced exploration and increased exploitation of the learned policy.

```
Episode 478/500 - Reward: 35, Epsilon: 0.0929
Episode 479/500 - Reward: 142, Epsilon: 0.0925
Episode 480/500 - Reward: 341, Epsilon: 0.0920
Episode 481/500 - Reward: 256, Epsilon: 0.0915
Episode 482/500 - Reward: 65, Epsilon: 0.0911
Episode 483/500 - Reward: 196, Epsilon: 0.0906
Episode 484/500 - Reward: 218, Epsilon: 0.0902
Episode 485/500 - Reward: 65, Epsilon: 0.0897
Episode 486/500 - Reward: 153, Epsilon: 0.0893
Episode 487/500 - Reward: 370, Epsilon: 0.0888
Episode 488/500 - Reward: 160, Epsilon: 0.0884
Episode 489/500 - Reward: 273, Epsilon: 0.0879
Episode 490/500 - Reward: 138, Epsilon: 0.0875
Episode 491/500 - Reward: 52, Epsilon: 0.0871
Episode 492/500 - Reward: 153, Epsilon: 0.0866
Episode 493/500 - Reward: 158, Epsilon: 0.0862
Episode 494/500 - Reward: 100, Epsilon: 0.0858
Episode 495/500 - Reward: 305, Epsilon: 0.0853
Episode 496/500 - Reward: 139, Epsilon: 0.0849
Episode 497/500 - Reward: 311, Epsilon: 0.0845
Episode 498/500 - Reward: 290, Epsilon: 0.0841
Episode 499/500 - Reward: 104, Epsilon: 0.0836
Episode 500/500 - Reward: 271, Epsilon: 0.0832
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Fig. 3 Training progress: episode rewards and decay in reinforcement epsilon

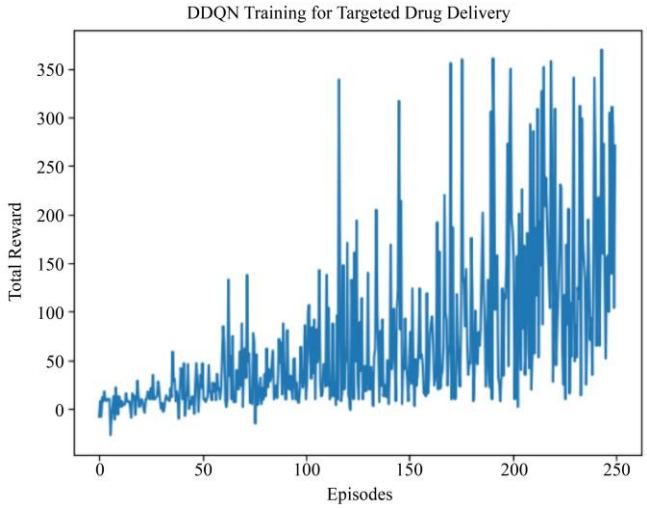

Fig. 4 Learning curve across 500 episodes

Figure 4 indicates the graph that shows DDQN training for targeted drug delivery. Rewards start low and unstable in early episodes but gradually increase, indicating the model learns effective strategies. By later episodes, higher rewards reflect improved optimization of the drug route and release rate.

6.3. Performance Metrics

6.3.1. Delivery Error Analysis

The delivery error is defined as the number of errors incurred when delivering the drug to the targeted site. Mathematically, it is defined by the ratio of overall error to the drug delivery error, which can be formulated as,

$$\mathrm{Del}^{\mathrm{err}} = \frac{\mathrm{App}^{\mathrm{err}} - \mathrm{Act}^{\mathrm{err}}}{\mathrm{Act}^{\mathrm{err}}} \quad (8)$$

Where, $\mathrm{Del}^{\mathrm{err}}$ denotes the delivery error, $\mathrm{App}^{\mathrm{err}}$ and $\mathrm{Act}^{\mathrm{err}}$ denotes the approximate and actual error, respectively.

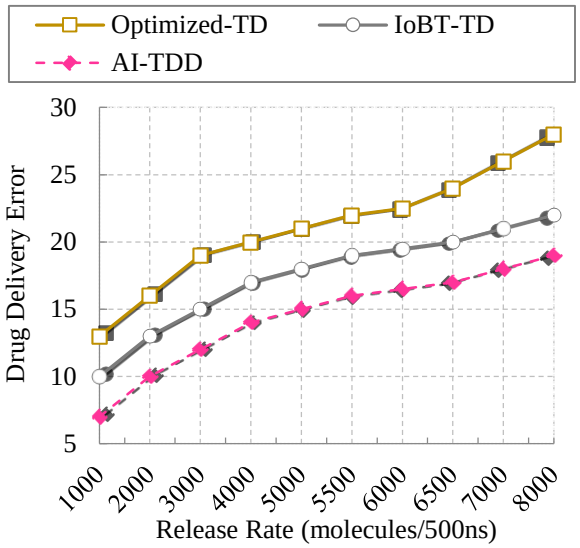

Fig. 5 Drug delivery error Vs Release rate

Figure 5 compares the medication delivery error rate between the suggested and current works. The graphic makes it quite evident that when the release rate rises, so does the medication delivery rate. Compared to the other two existing efforts, the suggested AI-TDD achieves a lower drug delivery error. The suggested AI-TDD reduces the likelihood of drug waste and ensures good control over the drug control method by performing the adaptive drug release process using a reinforcement algorithm called DDQN with appropriate metrics like biomarker concentration, dynamic location, and dynamic distance. On the other hand, despite designing an adaptive drug release model, the current works Optimized-TD and IoBT-TD fail to take into account crucial measurements and intelligence, which results in inadequate control and drug waste. Overall, the existing works are more prone to drug delivery error than the proposed work.

When the release rate is increased to 8000 molecules/500 ns, the current works IoBT-TD and Optimized-TD obtain drug delivery error rates of 22 and 28, respectively, whereas the suggested AI-TDD achieves 19, according to the numerical data from the graphical analysis above. There is a 3–9 lower difference between the projected and current medication delivery error rate studies.

6.3.2. RMSE Analysis

The Root Mean Square Error (RMSE) is defined as the estimation of drug delivery time error over the simulation replication time steps. The formulation of RMSE is provided below,

$$\text{RMSE} = \sqrt{\frac{\sum_{c=1}^{\propto} \tau^2(c)}{\propto}} \quad (9)$$

Where $\tau \propto$ is the time steps of simulation replications, τ is the delivery time error of the c-th replication.

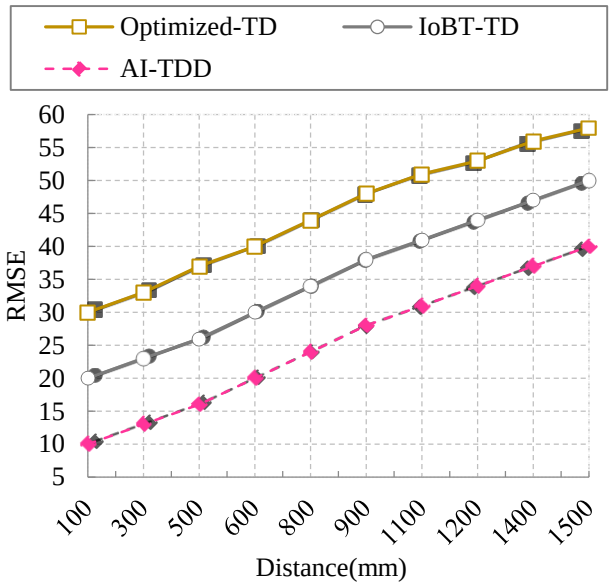

Fig. 6 Distance Vs RMSE

Figure 6 compares the proposed AI-TDD's RMSE rate to previous efforts. The RMSE rises as the distance increases, as the image illustrates. Additionally, the suggested approach performs better than the current model in terms of attaining lower RMSE. The primary cause of this lower RMSE is that the suggested work uses the DDQN algorithm to pick the best option among the obstruction paths while taking into account parameters like blood flow, blood velocity, position, and direction. The suggested work reduces the Issue of greater RMSE by calculating the best flow. However, IoBT-TD and Optimized-TD, the current works, do not have optimum path selection, which lowers the medication success rate and raises the RMSE compared to the suggested work.

When the distance is increased to 1500 millimeters, the current works IoBT-TD and Optimized-TD reach 50 and 58 drug RMSE, respectively, whereas the suggested AI-TDD achieves 40, according to the numerical findings from the graphical analysis above. There is a 10–18% lower discrepancy between the suggested and current medication delivery error rate studies.

6.3.3. Drug Release Rate Analysis

The drug release rate is defined as the number of drugs released when they reach the targeted site. Typically, the drug release rate is computed based on the disease severity and patients' conditions. The formulation of the drug release rate is provided below,

$$\text{DRR} = \text{Tot}^{\text{am}} - \text{rel}^{\text{am}} \quad (10)$$

Where DRR denotes the drug release rate, Tot^{am} denotes the total amount of drugs stocked in the nanomachine, and rel^{am} denotes the amount of drug released.

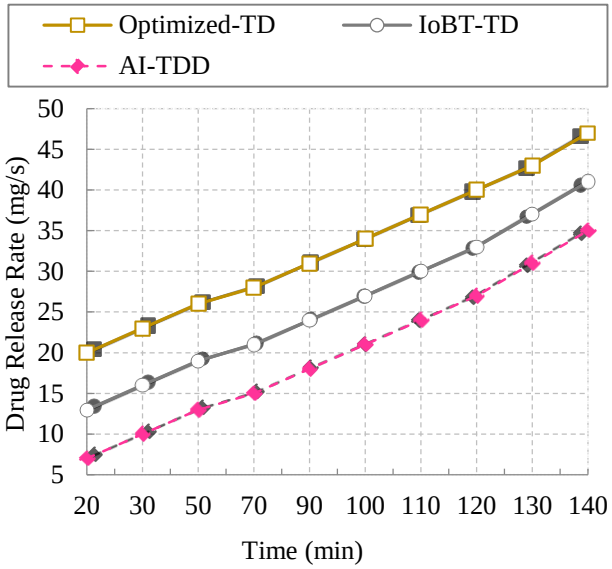

Fig. 7 Time Vs Drug release rate

Figure 7 compares the medication release rates of the planned AI-TDD study with those of the current studies. The line plot indicates that as time grew, so did the medication release rate. Despite the steady increase in duration, our suggested approach produces a lower drug release rate. The use of the DDQN-based adaptive release method resolves the problem of drug waste. However, despite their adaptive drug release capabilities, the current works, including IoBT-TD and Optimized-TD, lack optimal route selection, which results in a greater drug release rate than the suggested work. When the duration is increased to 140, the current works IoBT-TD and Optimized-TD obtain drug release rates of 41 mg/s and 47 mg/s, respectively, but the suggested AI-TDD achieves 35 mg/s, according to the numerical data from the above graphical analysis. There is a disparity of 6–12 mg/s between the projected and current medication delivery error rate studies.

6.3.4. Drug Reception Rate Analysis

The drug reception rate is defined as the amount of drug received by the targeted site. The drug reception rate must be higher when the release rate is higher.

Figure 8 presents a study of the medication reception rate for both the proposed AI-TDD and previous efforts. It is evident from the graphic that medication reception increases when the release rate is progressively raised. Accordingly, when the release rate is raised, our suggested approach achieves a larger drug reception rate. The main factor contributing to the suggested work's increased medication reception rate is its efficient target identification and route

delivery, respectively, which uses metrics like vessel pore size, cell density, and blood vessel perfusion status (i.e., blood, pressure, blood velocity, and red blood cell concentration) to enable precise localization, which in turn increases the drug release rate.

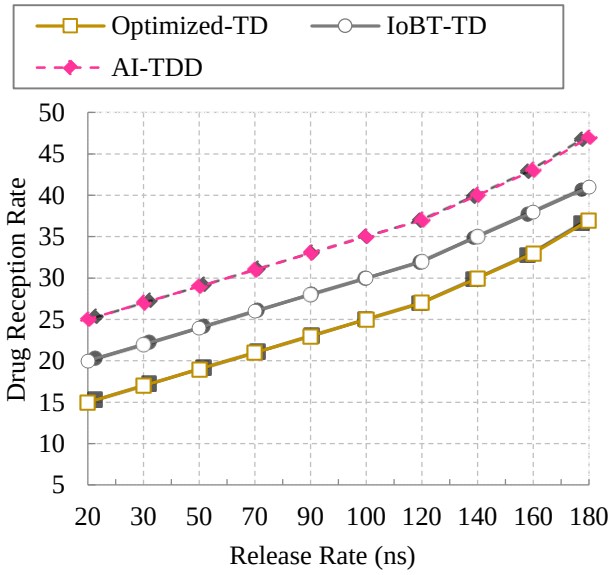

Fig. 8 Release rate Vs Drug reception rate

IoBT-TD and Optimized-TD, on the other hand, lack a superior target identification approach, which lowers their localization rate and results in a poor drug reception rate.

When the release rate is maximized to 180 ns, the current works, IoBT-TD and Optimized-TD obtain drug reception rates of 41 and 37, respectively, whereas the suggested AI-TDD achieves 47, according to the numerical data from the graphical analysis above. The suggested and current studies on medication delivery error rate varied by 6–10%.

6.3.5. Research Summary

The planned work's comprehensive research overview is given in this section. By using route administration, target localization, optimum route selection, and adaptive drug release techniques, the suggested work lowers the energy consumption rate, drug delivery error rate, and raises the drug delivery success rate. To achieve more intelligence and automated control, such approaches are structured according to machine learning, optimization, and reinforcement learning algorithms, respectively. Table 4 below displays the average quantitative analysis for the proposed and existing work, while the figures from (5) to (8) give the qualitative analysis in the form of a graphical depiction to help visualize the full impact of the planned work.

Table 4. Average results of proposed Vs Existing works

Metrics		AI-TDD	IoBT-TD	Optimized-TD	Difference
Release Rate	Drug Delivery Error	86	120.5	143.5	23-57.5
Distance	RMSE	25.3	35.3	45	9.7-19.7
Time	Drug Release Rate	20.1	26.1	32.9	6.8-12.8
Release Rate	Drug Reception Rate	34.7	29.6	24.7	4.9-10

7. Conclusion

The absence of intelligence, poor path selection, and ineffective drug delivery rates are the utmost pitfalls of the existing works. The aforementioned issues are resolved by adopting the proposed AI-based DDQN intelligent nanomachine control system. The AI-TDD model outperforms existing methods, Optimized-TD and enhances targeted drug delivery efficiency, minimizes side effects, and improves patient outcomes. The adaptive drug release model is framed by considering metrics such as biomarker concentration, dynamic location, and dynamic distance using the DDQN algorithm to enable robust drug delivery control and reduce drug wastage. The validation of the proposed work is evaluated using metrics such as drug delivery error, RMSE, drug release rate, and drug reception rate. The results show that the proposed model reflects better performance than the existing models (IOBT-TD and Optomized-TD). AI-driven optimization in drug delivery significantly reduces drug wastage and increases precision, making AI-TDD a promising method for molecular communication-based targeted drug delivery.

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