INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES
[ISSN: 0975-4725; CODEN(USA): IJPS00]
Journal Homepage: https://www.ijpsjournal.com

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Review Article

AI in Drug Delivery

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ARTICLE INFO

Published: 23 Aug 2025

Keywords:
Artificial intelligence; Drug delivery systems; Machine learning; Personalized medicine; Nanotechnology; Clinical trials; Predictive modeling; Precision medicine

DOI:
10.5281/zenodo.16933851

ABSTRACT

Drug delivery systems (DDS) have evolved significantly to improve therapeutic efficiency, stability, and patient compliance, yet challenges such as poor targeting, variability in patient responses, and high development costs persist. Artificial intelligence (AI) is emerging as a transformative tool to address these limitations by leveraging data-driven approaches across formulation, nanotechnology, targeted therapies, controlled release, and personalized medicine. AI algorithms, including machine learning, deep learning, and molecular simulations, enable predictive modeling of drug–carrier interactions, optimization of formulation parameters, and real-time clinical monitoring. Integration of AI into clinical trials further enhances patient recruitment, adherence monitoring, and adaptive trial designs, while regulatory bodies are beginning to establish frameworks for AI adoption. Despite challenges such as data quality, interpretability, and ethical concerns, the potential of AI-driven DDS is immense. Future trends point toward the integration of AI with blockchain, 3D printing, Internet of Medical Things (IoMT), digital twins, and quantum computing, offering patient-specific and cost-effective therapeutic solutions. This review underscores AI as not merely an incremental tool but a paradigm shift in drug delivery, paving the way for precision medicine and improved healthcare outcomes.

INTRODUCTION

Drug delivery systems (DDS) represent one of the most dynamic areas in pharmaceutical sciences, aiming to optimize therapeutic outcomes by improving drug stability, solubility, pharmacokinetics, and targeted release. Traditional DDS, while effective in many cases, often face significant challenges including poor site-specific targeting, unpredictable pharmacodynamics, high variability in patient response, and undesirable side effects. These limitations have fueled the demand for novel approaches that can accelerate development, personalize treatment, and improve patient compliance [(1).]

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Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Artificial intelligence (AI) has emerged as a transformative tool in healthcare and biomedical sciences. Initially applied to medical imaging, diagnostics, and genomics, AI now plays a significant role in pharmaceutical research. Its integration into drug delivery is particularly promising, as it enables predictive modeling of drug–excipient interactions, real-time optimization of formulations, and improved clinical decision-making[2].

The intersection of AI with drug delivery is reshaping how formulations are designed and evaluated. Unlike conventional trial-and-error methods, AI-based models leverage big data and computational power to predict drug solubility, bioavailability, and controlled release kinetics before laboratory validation. This accelerates the research timeline and reduces costs significantly [3]. Moreover, with the growing emphasis on precision medicine, AI-driven strategies are being used to tailor drug delivery to individual patients based on genetic, metabolic, and physiological variations [4].

The scope of this review is to provide a comprehensive understanding of the role of AI in drug delivery systems. It will explore how AI differs from its use in drug discovery, its applications in formulation science, nanotechnology, targeted therapies, personalized medicine, and controlled release systems. Additionally, computational tools, regulatory aspects, advantages, limitations, and future perspectives of AI in drug delivery will be discussed.

This review highlights AI's transformative potential in addressing long-standing challenges in pharmaceutical formulation and its critical role in the future of healthcare.

2. Overview of Artificial Intelligence in Healthcare

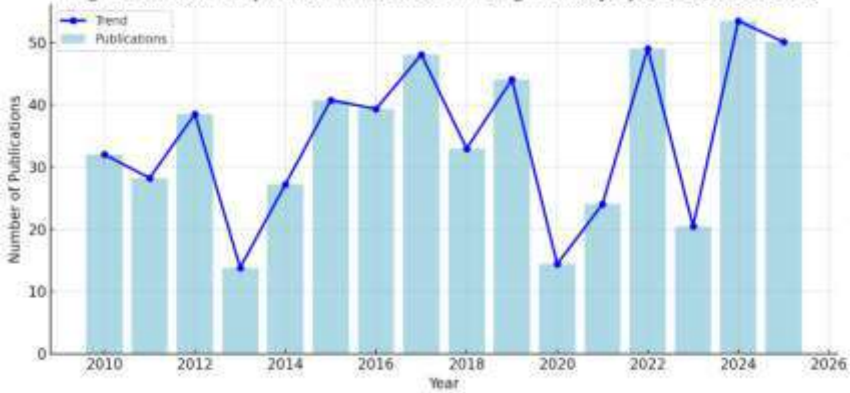
Artificial intelligence (AI) refers to computational systems capable of performing tasks that typically require human intelligence, such as learning, reasoning, pattern recognition, and decision-making. In healthcare, AI has rapidly evolved from being a theoretical concept to a practical tool that is now widely integrated into diagnostics, therapeutics, and clinical decision support systems [5].

2.1 Definitions and Core Concepts

AI encompasses multiple subfields, including **machine learning (ML)**, which focuses on algorithms that improve automatically through experience, and **deep learning (DL)**, a subset of ML based on artificial neural networks (ANNs) designed to mimic the human brain's processing structure [6]. Other important approaches include reinforcement learning, natural language processing (NLP), and computer vision, all of which have applications in biomedical sciences [7].

- **Machine Learning (ML):** Uses algorithms such as Support Vector Machines (SVM), Random Forests, and Gradient Boosting to identify patterns in large datasets.
- **Deep Learning (DL):** Employs multi-layered neural networks for tasks such as image recognition, molecular structure prediction, and clinical data interpretation.
- **Artificial Neural Networks (ANNs):** Inspired by the brain's structure, ANNs enable AI to simulate nonlinear and complex relationships in biomedical data [8].

Figure 1. Trend Graph of AI Publications in Drug Delivery Systems (2010-2025)



2.2 Historical Background

The concept of AI in healthcare dates back to the 1970s with early expert systems such as MYCIN, designed to support clinical decision-making in infectious disease management [9]. However, limited computational power and lack of digital data restricted widespread adoption. The explosion of big data in genomics, electronic health records (EHRs), and biomedical imaging—along with advancements in computing—has since enabled AI to flourish [10].

Over the past two decades, AI applications have grown exponentially across medical fields including **radiology**, **pathology**, **genomics**, **epidemiology**, and **pharmaceutical research** [11]. Its ability to handle multi-modal datasets (clinical records, molecular data, and imaging) makes AI particularly suited to addressing complex healthcare problems.

2.3 Advantages of AI in Biomedical Sciences

AI provides several advantages over traditional computational and statistical models:

- **Handling Large Datasets:** AI can process terabytes of biological and clinical data for meaningful insights [12].
- **Pattern Recognition:** AI identifies hidden patterns in multi-dimensional datasets, which may not be visible to human experts [13].
- **Predictive Modeling:** AI forecasts treatment outcomes, disease progression, and drug interactions with higher accuracy than conventional models [14].
- **Personalization:** AI integrates patient-specific data (genomic, proteomic, and metabolomic information) to optimize therapies.
- **Automation:** AI automates repetitive tasks, reducing healthcare costs and time burdens.[14]

2.4 AI in Pharmaceutical Sciences

In drug development, AI is used to accelerate **target identification**, **compound screening**, and **drug repurposing**. However, its role in **drug delivery** is gaining increasing attention because delivery systems often involve complex interactions between drugs, carriers, and biological systems. AI models can predict drug solubility, stability, and release kinetics, thereby reducing the reliance on costly trial-and-error approaches.

Thus, AI has emerged not only as a supportive tool in healthcare but also as a transformative enabler that bridges the gap between complex biomedical problems and effective therapeutic solutions.[15]

1. AI in Drug Discovery vs. Drug Delivery

Artificial intelligence (AI) has gained significant attention across pharmaceutical sciences, particularly in **drug discovery** and **drug delivery**. Although these two areas are closely related, they represent distinct stages of the pharmaceutical pipeline, each with its own challenges, datasets, and applications. Understanding their differences is crucial to appreciating the unique role of AI in advancing **drug delivery systems (DDS)**.

3.1 Drug Discovery: Role of AI

Drug discovery involves the identification of novel therapeutic candidates by screening large libraries of chemical compounds against specific biological targets. This process is traditionally expensive, time-consuming, and associated with high attrition rates [16]. AI has transformed this field by enabling:

- **Virtual Screening & De Novo Drug Design:** Machine learning (ML) and deep learning (DL) models identify promising molecules, reducing the need for extensive wet-lab screening.
- **Target Identification:** AI integrates omics data (genomics, proteomics, metabolomics) to uncover new therapeutic targets.
- **Drug Repurposing:** AI analyses clinical trial data and electronic health records to repurpose existing drugs for new indications.
- **Toxicity Prediction:** AI algorithms predict off-target effects and toxicity profiles, reducing late-stage failures.[17]

Thus, AI has revolutionized discovery by **reducing cost, accelerating timelines, and enhancing success rates** in the early phases of drug development.

3.2 Drug Delivery: Role of AI

While drug discovery focuses on finding *what* molecule can be used as a therapeutic, drug delivery is concerned with *how* that molecule is administered effectively, safely, and efficiently. AI applications in this domain include:

- **Formulation Optimization:** Predicting solubility, dissolution, stability, and excipient compatibility for oral, parenteral, and topical formulations.
- **Nanotechnology Integration:** Designing and optimizing nanoparticles, liposomes, and micelles with AI to improve targeting efficiency [18].
- **Targeted Delivery:** AI-driven models predict drug penetration through physiological barriers (e.g., blood–brain barrier) and optimize site-specific release
- **Controlled Release Systems:** AI predicts release kinetics in sustained and pulsatile delivery, enabling smarter implantable and transdermal systems[19]

Drug delivery is inherently more **multidimensional** than discovery, as it requires consideration of pharmacokinetics, pharmacodynamics, patient-specific variability, and complex material–drug–biological interactions. AI excels at capturing such complexity through data-driven models.[20]

3.3 Why AI is Particularly Useful in Drug Delivery

The utility of AI in drug delivery lies in several key aspects:

1. **Data Integration:** AI integrates heterogeneous data (molecular descriptors, patient data, material properties) to provide holistic insights.
2. **Predictive Accuracy:** Complex interactions between drugs, carriers, and biological

systems are modeled with higher precision compared to traditional statistical approaches.

3. **Reduction in Trial-and-Error:** Traditional DDS development involves iterative experiments; AI streamlines this by predicting outcomes in silico.
4. **Personalization:** With advances in pharmacogenomics, AI enables tailoring of delivery systems to individual patient needs, improving efficacy and reducing adverse reactions[21]

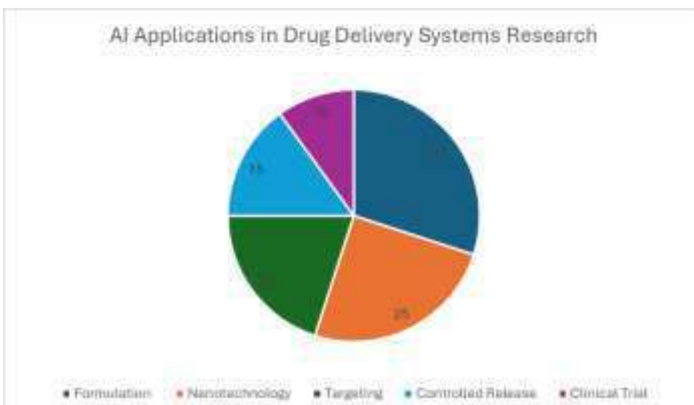
3.4 Integration into Formulation Science and Personalized Medicine

The boundary between drug discovery and delivery is increasingly blurred. AI is facilitating a **continuum** where early-stage discovery feeds directly into delivery system design. For instance, an AI-identified drug candidate may undergo simultaneous optimization for solubility, encapsulation, and release kinetics. Furthermore, AI-driven **digital twins**—virtual models of patients—are being explored to test and optimize delivery regimens in silico before clinical validation [22].

Thus, while drug discovery answers the "what" of therapeutics, drug delivery answers the "how," and AI is bridging both domains to accelerate translation into clinical practice.

4. Applications of AI in Drug Delivery

Artificial intelligence (AI) has emerged as a transformative technology in the design, optimization, and evaluation of drug delivery systems (DDS). Its applications span across **formulation science, nanotechnology, targeted therapies, personalized medicine, and controlled release systems**, each of which plays a critical role in modern therapeutics.



4.1 AI in Formulation Development

Formulation development traditionally relies on **trial-and-error** approaches, which are time-intensive and resource-demanding. AI provides predictive models that significantly reduce experimental burden.

- **Solubility and Stability Prediction:** Machine learning algorithms such as Support Vector Machines (SVMs) and Random Forests can predict the aqueous solubility and chemical stability of active pharmaceutical ingredients (APIs) based on molecular descriptors [23].
- **Excipient Selection and Compatibility:** AI models optimize excipient choice by analyzing large formulation datasets, predicting potential incompatibilities, and minimizing degradation pathways [24].
- **Drug Release Kinetics:** Neural networks have been applied to model dissolution

profiles, bioavailability, and pharmacokinetic parameters, enabling more accurate prediction of in vivo behavior [25].
- **High-Throughput Screening:** AI-driven platforms can process combinatorial formulation libraries to identify optimal compositions faster than conventional design of experiments (DoE) methods [26].

By integrating computational modeling with experimental validation, AI accelerates formulation development while reducing costs and improving success rates.

4.2 AI in Nanotechnology-Based Drug Delivery

Nanotechnology has revolutionized drug delivery by enabling **nanocarriers** such as nanoparticles, liposomes, micelles, and dendrimers. AI enhances this domain by:

- **Nanoparticle Design:** Machine learning predicts nanoparticle size, morphology, and zeta potential, which influence drug loading and release efficiency.
- **Surface Functionalization:** AI models evaluate ligand–receptor interactions, improving targeting efficiency in cancer nanomedicine and gene delivery
- **Optimization of Liposomes and Micelles:** Deep learning algorithms simulate encapsulation efficiency, stability, and pharmacokinetics of lipid-based carriers.
- **Nanotoxicity Prediction:** AI-based classifiers predict the cytotoxicity and immunogenicity of nanocarriers, addressing safety concerns [27].

For example, convolutional neural networks (CNNs) have been applied to analyze electron microscopy images of nanoparticles, providing real-time feedback on particle uniformity.

4.3 AI in Targeted Drug Delivery

Targeted delivery aims to ensure therapeutic agents reach specific tissues or cells while minimizing systemic side effects. AI enhances precision in:

- **Cancer Therapy:** AI models integrate tumor microenvironment data to optimize nanoparticle accumulation via the enhanced permeability and retention (EPR) effect [28].
- **Blood–Brain Barrier (BBB) Penetration:** Predictive models assess drug permeability across the BBB, a major obstacle in central nervous system (CNS) drug delivery [29].
- **Stimuli-Responsive Systems:** AI helps design smart polymers that respond to pH, temperature, or enzymatic triggers for on-demand release [30].
- **Organ-Specific Targeting:** AI-driven molecular docking and pharmacokinetic simulations predict ligand modifications required for liver, lung, or cardiac targeting [31].

These applications highlight AI's potential to transform targeted therapies into safer, more effective treatments.

4.4 AI in Personalized and Precision Medicine

Personalized drug delivery is central to the future of therapeutics. AI leverages **patient-specific data** to optimize dosage and delivery methods:

- **Pharmacogenomics:** AI algorithms analyze genetic polymorphisms influencing drug metabolism (CYP450 enzymes, transporters), guiding individualized dosing.
- **Digital Twins:** Virtual patient models simulate treatment scenarios, allowing optimization of DDS before actual clinical use.

- **Wearable Devices and IoMT:** AI-enabled devices monitor patient responses in real time, adjusting drug delivery dynamically.
- **Adaptive Dosage Systems:** Smart insulin pumps and implantable devices use AI algorithms to regulate drug release based on physiological feedback [32].

This patient-centered approach reduces adverse effects and enhances therapeutic efficacy.

4.5 AI in Controlled Release Systems

Controlled release systems aim to maintain therapeutic drug levels over prolonged periods. AI enhances their design by:

- **Mathematical Modeling of Release Profiles:** ML algorithms predict sustained, pulsatile, and delayed release behaviors in polymer-based systems.
- **Implantable Devices:** AI-guided models optimize implant geometry, degradation rates, and drug diffusion dynamics.
- **Transdermal and Oral Systems:** Predictive models help in selecting polymers and membranes with desired permeability.
- **Smart Hydrogels and Polymers:** AI aids in designing materials that respond to environmental stimuli, ensuring precise control over drug release [33].

These applications bridge computational predictions with experimental validation, streamlining the design of advanced DDS.

5. Computational Tools and Algorithms in Drug Delivery

The success of artificial intelligence (AI) in drug delivery systems (DDS) depends heavily on the **computational tools and algorithms** used to analyze complex datasets and predict formulation outcomes. Modern DDS involves integrating data from chemistry, biology, pharmacology, and clinical sciences, requiring sophisticated models capable of handling multi-dimensional information.

5.1 Machine Learning Models in DDS

Support Vector Machines (SVMs)

SVMs are supervised learning models widely used for **classification and regression** problems. In DDS, SVMs predict drug solubility, permeability, and bioavailability based on molecular descriptors. They are also applied in identifying excipient compatibility and predicting nanoparticle stability.[34]

Random Forest (RF) Models

RF is an ensemble learning method that constructs multiple decision trees and combines their outputs. In DDS, RF has been used to predict pharmacokinetic parameters such as absorption, distribution, metabolism, and excretion (ADME) properties of drugs, as well as release kinetics from polymeric systems [35].

Gradient Boosting Machines (GBM)

GBM algorithms build sequential decision trees that improve prediction accuracy. In DDS, GBM models are employed to identify key factors influencing drug encapsulation efficiency and stability of nanocarriers [36].

5.2 Deep Learning and Neural Networks

Deep learning (DL) approaches—especially **artificial neural networks (ANNs)** and **convolutional neural networks (CNNs)**—play a central role in modeling nonlinear relationships in drug delivery.

- **ANNs:** Applied in predicting drug dissolution rates, oral bioavailability, and implant release profiles
- **CNNs:** Used for analyzing nanoparticle images, predicting morphology, and optimizing structural properties of nanocarriers
- **Recurrent Neural Networks (RNNs):** Model sequential drug release profiles and time-dependent pharmacokinetics [37].

These models provide higher predictive accuracy than classical statistical methods, particularly when handling high-dimensional datasets.

5.3 Molecular Dynamics (MD) Simulations and AI

Molecular dynamics simulations provide atomic-level insights into drug–carrier interactions. AI enhances MD simulations by reducing computational cost and improving predictive power.

- AI accelerates simulations of drug encapsulation in liposomes and micelles.
- Hybrid AI–MD frameworks predict polymer degradation rates and diffusion dynamics of drugs from controlled release systems.
- Deep reinforcement learning has been applied to explore optimal nanoparticle–cell membrane interactions, reducing the need for laborious wet-lab studies [38].

5.4 Bioinformatics and Cheminformatics in DDS

Bioinformatics and cheminformatics databases provide large-scale datasets that fuel AI-driven drug delivery research:

- **ChEMBL and PubChem:** Contain bioactivity and chemical data used to train models for solubility and stability prediction.
- **DrugBank and PharmGKB:** Provide pharmacogenomic data for personalized medicine-based DDS.
- **Protein Data Bank (PDB):** Structural datasets help in ligand-receptor modeling for targeted drug delivery [39].

AI leverages these databases to develop predictive algorithms for formulation optimization, drug targeting, and patient-specific therapy.

5.5 Integration of Computational Tools in DDS

The integration of machine learning models, deep learning, molecular simulations, and bioinformatics has enabled the development of end-to-end AI platforms for DDS. These platforms can:

- Simulate drug–carrier interactions.
- Optimize excipient and polymer choices.
- Predict release kinetics.
- Personalize treatment regimens.

Such computational ecosystems reduce dependence on trial-and-error experimentation and accelerate clinical translation.

6. AI in Clinical Trials and Regulatory Aspects

The clinical trial stage is one of the most expensive and time-consuming phases of drug development. Despite significant advances in drug discovery and delivery systems (DDS), **late-stage clinical failures** remain common due to inadequate efficacy, unforeseen toxicity, and patient variability. Artificial intelligence (AI) offers powerful tools to address these issues by improving patient recruitment, adherence monitoring, data analysis, and regulatory compliance.

6.1 AI-Driven Patient Recruitment and Stratification

Recruitment is a major bottleneck in clinical trials, often delaying timelines and inflating costs. AI streamlines this process by:

- **Analyzing Electronic Health Records (EHRs):** AI extracts and filters patient data to match eligibility criteria efficiently.
- **Predictive Analytics for Enrollment:** Machine learning models forecast recruitment challenges and optimize trial site selection.
- **Patient Stratification:** AI identifies patient subgroups based on genetics, biomarkers, or comorbidities, enabling precision-based trials.

For instance, IBM Watson Health has been used to improve cancer trial recruitment by rapidly matching patients to suitable protocols.[40]

6.2 Monitoring Patient Adherence and Outcomes

Non-adherence to therapeutic regimens is a major reason for trial failure. AI improves adherence by:

- **Wearable Devices & IoMT:** AI-enabled sensors track medication intake and physiological responses in real time.
- **Mobile Health (mHealth) Apps:** Applications use AI-based reminders, chatbots, and digital companions to enhance compliance.
- **Digital Biomarkers:** AI analyzes physiological signals (e.g., heart rate, glucose levels, mobility patterns) to provide objective measures of drug efficacy.[41]

These tools ensure real-time monitoring and data-driven adjustments, improving the reliability of DDS evaluation.

6.3 Role of AI in Data Management and Analysis

Clinical trials generate vast amounts of heterogeneous data (clinical, molecular, imaging, wearable device data). AI assists in:

- **Data Cleaning and Integration:** AI algorithms reduce errors in trial datasets and merge multi-modal information.
- **Predictive Modeling of Trial Outcomes:** AI forecasts trial success or failure based on early-phase data, potentially terminating unpromising studies early.
- **Adaptive Trial Designs:** AI allows trials to evolve dynamically (dose adjustments, patient inclusion criteria) while maintaining statistical integrity.[42]

6.4 Regulatory Challenges and Perspectives

The incorporation of AI into DDS introduces unique **regulatory considerations**.

- **FDA Perspective:** The U.S. Food and Drug Administration (FDA) has recognized AI's potential but emphasizes the need for transparency, reproducibility, and risk assessment in AI-driven systems [43]. The FDA's framework on "Good Machine Learning Practice" (GMLP) aims to guide developers in ensuring reliability.
- **EMA Perspective:** The European Medicines Agency (EMA) encourages AI for pharmacovigilance and clinical trial optimization but highlights challenges in data standardization and interpretability [44].
- **Data Integrity Issues:** Ensuring quality, consistency, and security of training datasets remains a priority. Poor data quality may lead to biased or unreliable AI predictions [45].
- **Black-Box Problem:** Many deep learning models lack interpretability, posing difficulties for regulatory approval where transparent reasoning is required [46].

6.5 Ethical and Legal Considerations

AI-driven DDS in clinical trials also raises ethical concerns:

- **Data Privacy:** Patient data used in AI models must comply with regulations such as **HIPAA** and **GDPR**
- **Bias and Equity:** Biased datasets can result in unequal treatment recommendations, disproportionately affecting minority groups
- **Liability Issues:** The question of accountability in AI-driven decision-making—whether it lies with clinicians, developers, or regulators—remains unresolved [47]

Fig: AI in Clinical Trials

7. Advantages of AI in Drug Delivery

1. **Accelerated Formulation Development**

- Predicts solubility, stability, and dissolution profiles before lab experiments
- Optimizes excipient compatibility and concentrations
- Models drug–carrier interactions using molecular simulations and ML[48]

2. **Reduced Research and Development (R&D) Costs**

- Decreases failed formulations through predictive modelling.
- Automates high-throughput screening of DDS.
- Reduces reliance on extensive animal/human testing with in silico studies [49].

3. **Higher Success Rates in Clinical Trials**

- Enables patient stratification and personalized dosing.
- Predicts adverse effects from pharmacogenomic and real-world datasets.
- Improves adherence monitoring via wearables and digital tools.[50]

4. **Improved Patient Compliance and Safety**

- Smart DDS devices (e.g., insulin pumps, implantables) adjust dosing automatically.
- Mobile health (mHealth) apps support adherence through AI reminders.
- Real-time monitoring of adverse effects using AI-enabled biomarkers [51].

5. **Enhanced Precision and Personalization**

- Pharmacogenomics-based AI dosing tailored to individual genetic makeup.
- Digital twin models simulate personalized treatment regimens.
- IoMT-based adaptive systems allow real-time dosage adjustment [52].

8. Challenges and Limitations of AI in Drug Delivery

While artificial intelligence (AI) has shown great promise in transforming drug delivery systems (DDS), several challenges and limitations remain that hinder its full-scale adoption.

8.1 Data Quality and Availability

- **Incomplete or biased datasets** can reduce the accuracy of AI predictions
- Clinical data are often fragmented across hospitals, making integration difficult.

- Limited availability of high-quality training data for niche DDS applications [53].

8.2 Interpretability and the "Black Box" Problem

- Deep learning models often lack **explainability**, making it difficult for scientists and regulators to trust predictions.
- Lack of transparency complicates regulatory approval processes
- Difficulty in identifying which parameters most influence predictions [54].

8.3 Ethical and Privacy Concerns

- Use of sensitive patient data raises **privacy and security issues**, requiring strict compliance with GDPR and HIPAA regulations
- AI algorithms may inherit **biases** from training data, leading to inequitable healthcare outcomes
- Ethical concerns regarding patient consent for AI-driven DDS trials [55].

8.4 Regulatory and Legal Challenges

- Current regulatory frameworks (FDA, EMA) are not fully equipped to assess AI-driven DDS
- Lack of **standardized guidelines** for AI model validation in pharmaceutical applications
- Legal liability remains unclear in cases of AI-driven clinical errors [56].

8.5 Technical and Infrastructure Limitations

- High computational costs and infrastructure requirements limit adoption in developing countries
- Integration of AI tools with existing laboratory and clinical workflows remains challenging
- Lack of interoperability between different AI platforms and health data systems [57].

9. Future Perspectives of AI in Drug Delivery

The integration of artificial intelligence (AI) into drug delivery systems (DDS) is still in its early stages, but rapid advances in computational science, material engineering, and digital health point toward an exciting future. Several emerging directions are expected to shape the next generation of AI-driven DDS.

9.1 Integration of AI with Blockchain Technology

- **Secure Data Handling:** Blockchain can provide decentralized, tamper-proof storage for sensitive patient data used in AI models
- **Data Sharing Across Institutions:** Blockchain facilitates secure sharing of clinical and pharmaceutical datasets for training AI without compromising privacy.
- **Regulatory Compliance:** Transparent audit trails in blockchain systems enhance trustworthiness and accountability of AI-driven DDS [58].

9.2 AI and 3D Printing in Drug Delivery

- Personalized Dosage Forms: AI-guided 3D printing enables creation of customized tablets, implants, and transdermal patches tailored to individual patient needs
- Complex Release Profiles: AI optimizes 3D-printed multilayer structures to achieve pulsatile or sustained drug release
- On-Demand Manufacturing: Integration of AI ensures rapid adjustment of 3D printing

parameters in response to clinical requirements [59].

9.3 AI with Internet of Medical Things (IoMT)

- **Real-Time Monitoring:** IoMT devices collect continuous patient data (heart rate, glucose, activity) for AI-based adaptive drug delivery
- **Closed-Loop Systems:** AI-enabled pumps and implants automatically adjust drug release based on physiological signals
- **Remote Healthcare:** Cloud-connected AI + IoMT supports remote monitoring and management of chronic diseases [60].

9.4 Quantum Computing for Predictive Drug Delivery

- **Enhanced Computational Power:** Quantum algorithms may solve optimization problems in DDS (e.g., predicting nanoparticle–cell interactions) faster than classical models
- **Simulation of Complex Biological Systems:** Quantum computing can model drug–biomaterial interactions at unprecedented accuracy
- **Synergy with AI:** Combining quantum computing with AI could exponentially accelerate drug formulation design and testing [61].

9.5 Digital Twins in Personalized Medicine

- **Virtual Patient Models:** AI-driven digital twins simulate drug delivery in silico, predicting pharmacokinetics and pharmacodynamics for each patient.
- **Adaptive Therapy Planning:** Real-time data integration enables continuous adjustment of drug dosage and release strategies.
- **Clinical Decision Support:** Digital twins provide clinicians with patient-specific simulations before prescribing treatment [62].

9.6 Roadmap for Clinical Translation

For AI-driven DDS to reach full clinical application, the following steps are essential:

1. **Data Standardization** across healthcare systems to ensure consistent AI training.
2. **Explainable AI Models** to improve regulatory acceptance.
3. **Interdisciplinary Collaboration** between AI scientists, pharmaceutical researchers, clinicians, and regulators.
4. **Scalable Infrastructure** in both developed and developing nations to ensure equitable adoption [63]

10. Results and Discussion

The integration of AI into drug delivery has demonstrated measurable improvements in both preclinical and clinical settings**.** AI-driven predictive models have consistently shown superior accuracy compared to conventional trial-and-error methods in areas such as drug solubility, excipient compatibility, and release kinetics. For instance, machine learning–based algorithms such as Support Vector Machines (SVMs) and Random Forests have enabled early prediction of formulation stability, significantly reducing the number of experimental iterations required. Similarly, deep learning models, particularly convolutional neural networks (CNNs), have advanced nanoparticle characterization and targeting, enhancing the efficiency of nanomedicine development.

Clinical trial integration provides another layer of validation. AI-supported patient recruitment, stratification, and adherence monitoring have been shown to accelerate timelines and reduce attrition rates. Digital biomarkers and IoMT-based tools allow real-time data collection, creating feedback loops that optimize DDS performance in a clinical setting. These results highlight how AI not only reduces development costs but also bridges the gap between laboratory research and clinical translation.

However, challenges remain. Data quality, privacy concerns, and the "black-box" problem of AI models hinder regulatory acceptance. Ethical considerations, including patient consent and bias mitigation, remain unresolved in many applications. Despite these challenges, results from pilot studies and translational research indicate that the benefits of AI in DDS outweigh the limitations, with promising outcomes in oncology, neurology, and personalized therapy models.

In summary, the discussion reflects that while AI is not yet universally integrated into drug delivery pipelines**,** evidence strongly supports its potential to revolutionize therapeutic strategies**.** With ongoing improvements in explainable AI, regulatory frameworks, and interdisciplinary collaboration, AI-driven DDS is poised to become a cornerstone of precision medicine in the near future.

CONCLUSION

Drug delivery systems (DDS) are at the forefront of modern pharmaceutical innovation, yet they continue to face significant challenges including poor targeting, variable patient responses, high development costs, and lengthy clinical timelines. Artificial intelligence (AI) has emerged as a powerful tool to overcome these barriers by offering data-driven solutions that enhance formulation development, optimize nanotechnology-based carriers, enable targeted and personalized therapies, and improve controlled release systems.

Compared with drug discovery, where AI primarily accelerates target identification and molecule design, its role in drug delivery is broader, addressing the "how" of drug administration. AI empowers researchers to predict solubility, stability, bioavailability, and release kinetics; design nanocarriers with optimal morphology and targeting efficiency; and integrate patient-specific data into delivery strategies.

The applications of AI in clinical trials further extend its impact by improving patient recruitment, adherence monitoring, trial design, and regulatory compliance. While challenges such as data quality, black-box interpretability, ethical concerns, and infrastructure limitations persist, the benefits far outweigh the hurdles. The ongoing development of explainable AI models, regulatory frameworks, and secure data-handling solutions is expected to accelerate its integration into pharmaceutical practice.

Looking forward, the future of AI in DDS lies in its synergy with blockchain for secure data sharing, 3D printing for customized dosage forms, IoMT for real-time adaptive drug release, digital twins for personalized medicine, and quantum computing for high-precision predictive modeling. These advancements hold the potential to transform healthcare into a patient-centered, cost-effective, and efficient ecosystem.

In conclusion, AI represents not just an incremental improvement but a paradigm shifts in drug delivery sciences. Its success will depend on multidisciplinary collaboration between pharmaceutical scientists, clinicians, data scientists, engineers, and regulators. With continued innovation and careful integration, AI-driven DDS can revolutionize therapeutic outcomes and usher in a new era of precision medicine.

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HOW TO CITE: Saqlain Mirasaheb Mujawar, Sadiya Dastagir Ugare, AI in Drug Delivery, Int. J. of Pharm. Sci., 2025, Vol 3, Issue 8, 2562-2578. https://doi.org/10.5281/zenodo.16933851