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## Review Paper

# Role of Artificial Intelligence in Modern Pharmaceutical Formulation Development: Current Applications, Challenges, and Future Perspectives

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## ABSTRACT

Artificial Intelligence (AI) has emerged as a disruptive technology in pharmaceutical sciences, especially in formulation development. Traditional formulation strategies are largely empirical and trial-and-error in nature which are time-consuming, costly and often inefficient. AI includes machine learning (ML), deep learning (DL) and artificial neural networks (ANN) integration allows predictive modelling, optimization of formulation parameters and reduce experimental workload (Gunjal, 2025). AI based systems can predict Drug Excipients compatibility, Dissolution profiles, Stability and Critical Quality attributes efficiently accelerating the development process. Additionally, AI aids in the design of advanced drug delivery systems such as nanoparticles and controlled-release formulations by optimizing design parameters and enhancing therapeutic outcomes. Even with these advantages, challenges of lack of data, model explainability and regulatory approval remain significant barriers. But the ongoing advances and increasing adoption of AI in pharmaceutical industries show its strong potential to revolutionize formulation development. (Sartaj et al., 2025). This review provides a comprehensive overview of the applications of AI in pharmaceutical formulation, discusses the key techniques, highlights the applications in industry, and discusses the future perspectives. The article also highlights the existing research gaps and regulatory considerations to guide the future development in this fast-changing field. (Sartaj et al., 2025).

## INTRODUCTION

Artificial intelligence has been revolutionizing many different scientific fields, and we are

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gradually seeing the importance of this revolution in pharmaceutical sciences, including drug formulation or development. (Ali et al., 2024; Sartaj et al., 2025).

Pharmaceutical formulation development is one of the key aspects in the pharmaceutical field, as it involves designing and optimizing a dosage form to obtain safety, efficacy, stability along with good patient compliance as per the scenario or indication for treatment. It includes the selection of excipients, find optimal composition and characterization of physicochemical properties.

Formulation creation has historically mostly relied on empirical methods and trial-and-error testing, which are frequently labour-intensive, resource-intensive, and highly prone to failure. Conventional formulation techniques are severely limited by the growing complexity of therapeutic molecules, including poorly soluble chemicals, biologics, and targeted drug delivery systems. These difficulties call for the use of increasingly sophisticated and effective techniques that can manage complicated datasets and produce precise forecasts.

Artificial intelligence (AI) has become a potent instrument that has the potential to revolutionize the development of pharmacological formulations. AI is the term for computing systems that are capable of learning, reasoning, and making decisions—tasks that normally require human intelligence. AI makes it possible to find hidden patterns and connections between formulation variables and performance outcomes by utilizing massive datasets and complex algorithms. (Sartaj et al., 2025; Nithyanantham, Nair, and Nayak, 2025).

The use of AI in pharmaceutical sciences has grown significantly in recent years as a result of improvements in processing power, the accessibility of large amounts of data, and the creation of reliable algorithms. Artificial intelligence (AI)-driven models, such machine

learning (ML) and deep learning (DL), have shown great promise in terms of formulation characteristic prediction, medication delivery system optimization, and experimental burden reduction.

AI's capacity to reduce reliance on conventional trial-and-error techniques is one of its main benefits in formulation development. AI models can quickly screen a variety of formulation variables and forecast the best combinations, which speeds up development and lowers costs. AI also improves decision-making by offering data-driven insights that increase formulation precision and repeatability. The application of AI in pharmaceutical formulation is not without difficulties, despite these encouraging benefits. Significant obstacles to its widespread use include problems like the scarcity of high-quality datasets, the interpretability of the model, and regulatory concerns. Furthermore, interdisciplinary knowledge and infrastructure are needed to integrate AI with current pharmaceutical procedures. (Salunke, 2026; Tade et al., 2023).

The goal of this review is to give a thorough overview of how AI is used in the development of contemporary pharmacological formulations. It covers basic ideas, important applications, industrial significance, and regulatory issues. It also emphasizes the revolutionary potential of AI in enhancing pharmaceutical sciences by highlighting existing obstacles, identifying research gaps, and exploring future perspectives. (Solake, 2024; Kandhare et al., 2025; Tade et al., 2023).

## **2. Artificial Intelligence Basics in Pharmaceuticals**

### **2.1 Artificial Intelligence Overview**

The ability of robots to carry out tasks that normally require human intelligence, such as learning from data, identifying patterns, making judgments, and resolving challenging issues, is



known as artificial intelligence (AI). AI is mostly utilized in the pharmaceutical industry to evaluate massive datasets, find correlations between formulation variables, and make highly accurate predictions.

Algorithms that can handle both organized and unstructured data are used by AI systems to derive valuable insights. These systems are very adaptive to changing pharmacological issues because they learn continuously throughout time. A change from empirical experimentation to predictive modeling has been made possible by the incorporation of AI into formulation development, which has improved efficiency and shortened development times (Jiang et al., 2022; Gunjal, 2025).

## 2.2 The Use of Machine Learning

A branch of artificial intelligence called machine learning (ML) focuses on creating algorithms that can learn from past data and make predictions without the need for explicit programming. By determining correlations between formulation factors (such as excipient concentration, particle size, and processing conditions) and output responses (like drug release, stability, and bioavailability), machine learning plays a critical role in pharmaceutical formulation.

Three major categories can be used to group ML techniques:

- **Supervised Learning:**

This method uses labeled datasets with established input-output correlations to train models. It is frequently used to forecast formulation performance and medication release characteristics.

- **Unsupervised Learning:**

Used to find hidden groupings or patterns in data that don't have labels. This method works well for finding patterns in big datasets or grouping similar formulations.

- **Learning by Reinforcement:**

a method of learning in which models use feedback and trial methods to increase performance. It has the potential to improve formulation processes, although being less often employed.

ML algorithms greatly reduce the requirement for substantial laboratory experiments by enabling quick screening of formulation factors. (Sartaj et al., 2025; Dangeti, Bynagari, and Vydani, 2023).

## 2.3 Deep Learning

Deep Learning (DL) is a sophisticated branch of machine learning that models complicated and nonlinear interactions using multi-layered artificial neural networks. DL is very good at managing big, complicated datasets, which makes it ideal for use in pharmaceutical applications. DL models can process high-dimensional data in formulation development, including molecular structures, imaging data, and process parameters, to forecast formulation results.

In tasks including drug release prediction, stability modeling, and drug delivery system optimization, these models have proven to perform better.

Deep learning's primary benefit is its capacity to automatically extract features from unprocessed data, doing away with the requirement for human feature engineering. (Prusty and Panda, 2024; Đuriš, Kurćubić, and Ibrić, 2021; Yang et al., 2018).

## 2.4 Synthetic Neural Networks

Computational models called Artificial Neural Networks (ANNs) are modeled after the composition and operations of the human brain. They are made up of layers of interconnected nodes, or neurons, that process incoming data and produce predictions for the output. Because ANNs can represent nonlinear connections between



variables, they are frequently utilized in the creation of pharmacological formulations. They have been effectively used to forecast stability results, dissolving profiles, and tablet characteristics.

Typical components of an ANN model include:

- Formulation variables in the input .
- Processing and learning layers that are hidden.
- The output layer (anticipated reaction) .

ANNs are powerful because of their excellent predicted accuracy and adaptability, particularly when working with complicated datasets.(Kovács et al., 2021; Das, Dey, and Nayak, 2021).

## 2.5 Preprocessing and Data Requirements

The quantity and quality of data used for training have a significant impact on how well AI models function. Data in pharmaceutical formulation can comprise excipient properties, processing parameters, drug physicochemical properties, and experimental results.

Important data preparation procedures include:

- Data Cleaning: Eliminating mistakes and discrepancies Normalization is the process of scaling data to ensure consistency.
- Feature Selection: Determining pertinent characteristics .
- Validation: Ensuring the precision and dependability of the model. Unreliable models and erroneous forecasts might result from inadequate or low-quality data.

For AI to be implemented successfully, strong data management and preprocessing are therefore crucial.(Nesterov, 2023; Singh, 2025).

## 2.6 AI's Significance in the Pharmaceutical Sector

AI offers the following benefits for developing pharmaceutical formulations:

- Capacity to manage intricate and substantial datasets .

- A decrease in the amount of work involved in experiments.

- Increased forecast precision.
- Quicker decision-making .

Because of these advantages, AI is a vital tool in contemporary pharmaceutical research, facilitating the creation of more inventive and effective drug compositions.(Sartaj et al., 2025; Sri, 2025; Vora et al., 2023).

## 3. Using Artificial Intelligence to Develop Pharmaceutical Formulations

Pharmaceutical formulation development has benefited greatly from artificial intelligence's ability to facilitate data-driven decision-making, optimization, and predictive modeling. These applications improve formulation efficiency and accuracy while drastically reducing development time, cost, and experimental workload.

### 3.1 Prediction of Drug-Excipient Compatibility

Drug–excipient compatibility is a critical factor in formulation development, as interactions between active pharmaceutical ingredients (APIs) and excipients can lead to instability, reduced efficacy, or degradation.

Compatibility assessments have historically involved laborious. Experimental methods including chromatographic analysis, Fourier transform infrared spectroscopy(FTIR),and differential scanning calorimetry (DSC).

By examining physicochemical characteristics, molecular structures, and historical records, AI-based models can forecast possible interactions between medications and excipients.

Patterns and correlations that might not be seen using traditional techniques are found using machine learning algorithms.

These forecasting talents aid in:

- Early detection of incompatible excipients.
- A decrease in the rates of formulation failure.
- Increased drug product stability and shelf life.



As a result, AI speeds up the formulation design process and reduces the requirement for lengthy experimental screening.(Sartaj and others, 2025).

### 3.2 Optimization of Formulation

To obtain desired product qualities, formulation optimization entails figuring out the best mix of excipients and process parameters. Traditional optimization techniques, such as Design of Experiments (DoE), can be resource-intensive and necessitate several experimental runs. By analyzing several factors at once, AI methods like genetic algorithms and artificial neural networks allow for quick optimization. These models are able to forecast how formulation variables will affect outcomes like stability, bioavailability, and drug release. AI has several important benefits for formulation improvement, such as:

- A decrease in the quantity of experiments .
- Quicker determination of the best formulations.
- Increased accuracy and consistency.

AI-driven optimization is especially helpful for complicated formulations with nonlinear variable interactions that are challenging to model with conventional techniques.(Yadav and others, 2025).

### 3.3 Forecasting Drug Release and Dissolution Characteristics

Pharmaceutical formulations' therapeutic efficacy is influenced by important factors such as drug release and dissolving behavior. Conventional techniques for assessing dissolution profiles need a great deal of time-consuming in vitro experimentation.

By examining formulation composition, physicochemical characteristics, and process factors, AI models are able to forecast drug release kinetics. Accurate release profile prediction is made possible by machine learning algorithms that can create correlations between input factors and

dissolution results.

Applications consist of:

- The creation of formulations with controlled release.
- Forecasting the behavior of immediate versus sustained release.
- Improvement of dissolving properties .

This predictive ability speeds up formulation development and lessens reliance on repeated dissolution tests.(Zaborenko and others, 2019) .

### 3.4 Estimating Shelf Life and Predicting Stability

To ascertain the shelf life and storage conditions of pharmaceutical items, stability studies are crucial. Long-term research in a variety of environmental settings is necessary for conventional stability testing, which can postpone product development. By evaluating past stability data and environmental variables like temperature, humidity, and light exposure, AI-based methods can forecast degradation routes and shelf-life. In a shorter amount of time, these models can replicate long-term stability results.

Advantages consist of:

- Less extensive stability studies are required.
- Quicker deadlines for regulatory submissions.
- Enhanced dependability of the product .

For medications with intricate degradation processes, AI-driven stability prediction is especially beneficial.Shingare (2026).

### 3.5 Creation of Solid Dosage Forms

The most popular pharmaceutical items are solid dose forms like tablets and capsules. Optimizing factors including hardness, friability, disintegration time, and compressibility is part of their development.

These characteristics can be predicted by AI models based on processing conditions and formulation makeup. Regression models and artificial neural networks are frequently



employed.

Applications consist of:

- Estimating the mechanical strength of tablets.
- Disintegration time optimization .
- Regulation of flow characteristics and compressibility.

This guarantees consistent performance and lowers product quality variability.(Kovács et al., 2021; Akseli et al., 2016).

### 3.6 AI in Advanced Drug Delivery Systems and Nanotechnology

Nanoparticles, liposomes, and polymeric carriers are examples of advanced drug delivery methods that necessitate exact control over a number of variables, including particle size, surface charge, and drug loading efficiency.

By evaluating intricate datasets and forecasting ideal formulation conditions, AI plays a critical role in optimizing these systems.

Relationships between formulation variables and delivery efficiency can be found using machine learning models.

Applications consist of:

- Optimization of the distribution and size of nanoparticles.
- Improving the bioavailability and targeting of drugs.
- Creating tailored and regulated drug delivery systems .

AI makes it possible to create more efficient and customized medication delivery systems, which enhances therapeutic results.(Kapoor and others, 2024).

### 3.7 Scale-Up and Process Optimization

The difficult process of scaling up a formulation from laboratory to industrial production frequently results in inconsistent product quality. AI can help with manufacturing process optimization and scale-up behavior prediction.

AI models can do the following by examining past production data and process parameters:

- Forecast process performance on a bigger scale.
- Determine important process variables.
- Cut down on manufacturing batch failures.

This guarantees a more seamless transition from research to commercial manufacturing.(Kalagnanam and others, 2022).

### 3.8 AI in Customized Healthcare

The goal of personalized medicine is to customize medication formulations according to each patient's unique attributes, including age, genetics, and medical condition.

AI makes it possible to analyze patient-specific data and create personalized formulas.Applications consist of:

- Dosage design tailored to each patient.
- Drug delivery system optimization.
- Better results from therapy .

A major development in contemporary healthcare is AI-driven personalized formulation (Patnaik et al., 2023; Ali et al., 2024; Gunjal, 2025; Sartaj et al., 2025).

### 4.AI Methods for Developing Pharmaceutical Formulations

Pharmaceutical formulation development u`ses a variety of AI tools to model intricate relationships, optimize formulation parameters, and make highly accurate predictions. Every technique has advantages and disadvantages that make it appropriate for particular uses.

#### 4.1 ANNs, or artificial neural networks

One of the most used AI methods in pharmaceutical formulation is artificial neural networks, or ANNs. They are made to resemble the interconnected layers of neurons that make up the human brain, both in terms of structure and function.

When modeling nonlinear interactions between formulation factors and responses, ANNs are



especially useful. They are employed in pharmaceutical applications to forecast outcomes including stability, tablet hardness, and drug release (Nagy et al., 2022).

Uses:

- Dissolution profile prediction.
- Optimizing the composition of the formulation.
- Complex medication delivery system modelling.

Advantages:

- Excellent forecast precision.
  - Capacity to manage nonlinear data.
  - Adaptability when simulating intricate systems.
- Limitations: Large datasets are necessary. Hard to decipher (black-box nature).

#### 4.2 SVMs, or support vector machines

Supervised learning models for regression analysis and classification are called support vector machines. SVM divides data into distinct groups by identifying the ideal border, or hyperplane. SVM is used in pharmaceutical formulation to categorize formulations according to their characteristics and predict formulation performance.

Uses:

- Stable versus unstable formulation classification.
- Forecasting the behavior of dissolution.
- Examining formulation datasets.

Advantages:-

- Suitable for tiny datasets.
  - Excellent classification task accuracy.
  - Sturdy against overfitting
- Restrictions:
- Limited capacity to scale for big datasets.
  - Needs meticulous parameter adjustment.

#### 4.3 The Random Forest

Multiple decision trees are used in the Random Forest ensemble learning technique to increase prediction accuracy.

It produces a more dependable outcome by combining the outputs of several models. Random Forest is frequently used in

pharmaceutical formulation to forecast formulation performance, stability, and drug release. (Pali and others, 2022).

Uses:

- Prediction of stability.
- Analysis of feature importance.
- Formulation variable optimization .

Advantages:

- Excellent precision and durability.
- Effectively manages big datasets.
- Lessens overfitting.

Limitations:

- Difficult interpretation.
- Computationally demanding.

#### 4.4 Algorithms for Genetics (GA)

Natural selection serves as the model for genetic algorithms, which are optimization strategies. To identify the best answers, they employ processes like selection, crossover, and mutation. By investigating several potential combinations, GA is used in formulation development to optimize formulation parameters. (Sgarro, Santoro, and Grilli, 2024).

Uses:

- Excipient concentration optimization.
- Optimization of process parameters.
- The creation of formulations with controlled release .

Advantages:

- Effective at resolving challenging optimization issues.

- Able to manage several variables at once .

Limitations:

- Needs a lot of processing power.
- If improperly constructed, it might converge to local optima.

#### 4.5 k-Nearest Neighbors (k-NN)

k-NN is a straightforward machine learning technique for regression and classification. It

forecasts results by comparing them to nearby data points.

Uses:

- Categorization of formulation kinds.
- Forecasting using patterns of similarity .

Advantages:

- Easy to use and straightforward .
- There is no need for a training period.

Limitations:

- Noise-sensitive.
- Less effective when dealing with big datasets (Duch, Swaminathan, and Meller, 2007; Taha, 2024).

#### 4.6 Models of Deep Learning

Pharmaceutical research is increasingly using deep learning models, such as recurrent neural networks

(RNNs) and convolutional neural networks (CNNs).

Complex information like time-series data, chemical structures, and imaging data can be processed by these models.

Applications:

- Advanced drug delivery system modelling.
- Image-based analysis (e.g., particle size distribution).
- Prediction of complex formulation behavior.

Advantages:

- High performance with large datasets.
- Automatic feature extraction.

Limitations:

- Requires high computational power.
- Needs large datasets for training.

**Table1: Comparison of AI Techniques in Pharmaceutical Formulation**

Technique	Application	Advantages	Limitations
ANN	Drug release prediction	High accuracy	Needs large data
SVM	Classification	Works with small data	Limited scalability
Random Forest	Stability prediction	Robust	Complex interpretation
Genetic Algorithm	Optimization	Efficient	Computational cost
k-NN	Pattern recognition	Simple	Sensitive to noise
Deep Learning	Complex modeling	Powerful	High resource requirement

Summary:

The following factors determine whether AI technology is best:

- The dataset's nature.
- The formulation's complexity.
- The intended result (optimization vs. forecast).

When many AI algorithms are combined, performance and forecast accuracy are frequently enhanced.(Sartaj et al., 2025; Ali et al., 2024).

### 5.QbD, PAT, Industrial Applications, and AI vs. Conventional Methods

#### 5.1. A Comparison of Conventional and AI-Based Formulation Methods

The creation of pharmaceutical formulations has historically depended on empirical and trial-and-error methods. Although these approaches have proven successful, they frequently have drawbacks including high expense, lengthy development times, and poor efficiency. By providing predictive and data-driven approaches, artificial intelligence has greatly enhanced these procedures.

To find ideal conditions, conventional techniques like Design of Experiments (DoE) call for several experimental runs. AI-based methods, on the other hand, can evaluate big datasets and forecast results with little trial and error. In contrast to traditional approaches, which frequently analyze one or a

small number of variables at a time, AI also enables the simultaneous evaluation of several variables. Because of this, AI is especially useful for intricate formulations including nonlinear interactions.(Sartaj et al., 2025; Shingare, 2026; Joshi and Sheth, 2025).

Key Insights:

- AI drastically cuts down on formulation development time.
- Increases the precision and repeatability of predictions.
- Reduces the workload associated with experiments.
- Makes it possible to comprehend complex systems better.

AI thus signifies a paradigm change in the creation of pharmacological formulations.

## 6. AI's Industrial Use in Pharmaceutical Formulation

AI technologies are being used by the pharmaceutical sector more and more to boost productivity, cut expenses, and improve product quality. AI is being incorporated at several phases of manufacturing and formulation development.

### 6.1 Optimization of Processes

In order to optimize production processes, AI models examine manufacturing parameters including temperature, pressure, and mixing time. This results in decreased variability and increased efficiency.

### 6.2 Technology Transfer and Scale-Up

Changes in process dynamics can make it difficult to scale up a formulation from laboratory to industrial scale. AI can identify crucial parameters and forecast scale-up behavior, guaranteeing a seamless transition and lowering batch failures.

### 6.3 Quality Assurance and Control

By evaluating data from sensors and analytical tools, AI-based systems are able to track product quality in real time. This guarantees constant product quality and allows for the early discovery of deviations.

### 6.4 Automated Manufacturing

AI makes intelligent control systems possible, which promotes automation in the pharmaceutical industry.

Real-time process parameter adjustments using these devices increase productivity and decrease human involvement.(Ali et al., 2024; Rajesh and Elumalai, 2025; Niazi, 2023).

## 7. Quality by Design (QbD) using AI

A methodical approach to pharmaceutical development, Quality by Design (QbD) places a strong emphasis on comprehending and managing formulation and process factors to guarantee product quality.

AI improves QbD through:

- Finding Critical Quality Attributes (CQAs).
- Finding the Critical Process Parameters (CPPs).
- Modeling the connections between variables and results .

Better risk assessment and formulation robustness are made possible by AI-driven QbD techniques. AI can forecast how modifications to formulation or process factors would impact product quality by examining massive datasets.

This results in:

- Enhanced uniformity of the product.
- A decrease in variability .
- Improved adherence to regulations (Dawoud et al., 2023; Khodade and Jagannath, 2025; Zhu, 2025).



**Table 2: Comparison of Traditional and AI-Based Approaches**

Parameter	Traditional Methods	AI-Based Methods
Approach	Trial-and-error	Data-driven
Time	High	Low
Cost	High	Reduced
Accuracy	Moderate	High
Experimental Trials	Extensive	Minimal
Scalability	Limited	High

## 8. Combining Process Analytical Technology (PAT) with AI

To guarantee product quality, Process Analytical Technology (PAT) monitors and controls pharmaceutical manufacturing processes in real-time. By facilitating intelligent data analysis and decision-making, the integration of AI with PAT improves its capabilities.

AI-PAT Integration Applications:

- Monitoring formulation processes in real time.
- Forecasting process deviations Process control that is automated.

• Continuous manufacturing AI algorithms can provide real-time insights into process performance by analyzing data from PAT tools like spectroscopy and chromatography.

Advantages:

- Enhanced process effectiveness.
- A decrease in production errors.
- Improved product quality.
- Quicker decision-making.

Summary:

AI's incorporation into the creation of pharmaceutical formulations has greatly enhanced industrial procedures by:

- Increasing productivity and efficiency.
- Cutting expenses and time.
- Increasing the consistency and quality of the product.
- Supporting sophisticated regulatory frameworks.

AI offers a thorough approach to contemporary pharmaceutical manufacture when paired with

QbD and PAT. (Panda and Prusty, 2024; Rajesh and Elumalai, 2025).

## 9. Comprehensive Case Studies in Pharmaceutical Formulation Using AI

Numerous commercial and experimental research have shown how artificial intelligence can be used in the development of pharmaceutical formulations. These case examples demonstrate how AI can be used to improve formulation science's productivity, accuracy, and creativity.

### 9.1 Case Study 1: AI-Powered Tablet Formulation Optimization

The development of tablet formulations entails the optimization of several factors, including granulation parameters, compression force, and excipient concentration.

Conventional optimization takes a lot of time and experimentation. Artificial Neural Networks (ANN) were used in this study to optimize tablet composition. Among the input parameters were:

- Excipient concentration (binders, disintegrants).
  - The force of compression Granule size.
  - The measured output responses were:
    - The hardness of tablets
- Experimental data was used to train the ANN model, and further test formulations were used to validate it.
- The model accurately and successfully anticipated formulation outcomes.

Key Outcomes:

- A 50–60% decrease in experimental trials.



- Quicker determination of the ideal formulation composition.

- Enhanced consistency and reproducibility

Importance:

This study showed that AI can greatly speed up tablet development by successfully replacing conventional trial-and-error techniques. (Ghazwani and Hami, 2025; Singh et al., 2025; Bounab et al., 2025).

## 9.2 Case Study 2: AI in Nanoparticle Drug Delivery System Optimization

Precise control over variables including particle size, surface charge (zeta potential), and drug loading efficiency is necessary for nanoparticle-based drug delivery systems.

Bioavailability and therapeutic efficacy are directly impacted by these factors. In this instance, the formulation of nanoparticles was optimized using machine learning models, such as Random Forest and ANN.

Among the variables in the dataset were:

- The concentration of polymers.
- Ratio of drug to polymer.
- Temperature and stirring speed.

Relationships between these variables and formulation results were examined by the AI models.

Key Outcomes:

- Precise estimation of drug encapsulation effectiveness and particle size.
- Improving formulation characteristics to increase bioavailability.
- A decrease in the amount of work involved in experiments.

Importance:

AI's potential in cutting-edge drug delivery technologies was demonstrated by the effective design of nanoparticle systems with improved drug delivery performance. (Shen et al., 2025; Vengateswaran et al., 2025; Kapoor et al., 2024)

## 9.3 Case Study 3: AI-Powered Shelf-Life Estimation and Stability Prediction

Determining the shelf-life of medicinal items requires stability research. Conventional stability testing, however, necessitates long-term research in several environmental settings.

In this case study, historical stability data was used to train machine learning algorithms, such as:

- Conditions of humidity and temperature.
- Constants of degradation rate.
- Information about chemical stability.

The model calculated shelf life under different storage circumstances and forecasted degradation behavior.

Key Outcomes:

- Precise estimation of degradation kinetics.
  - A decrease in the requirement for long-term stability investigations.
  - Quicker deadlines for regulatory submissions
- Importance:

AI-based stability prediction drastically cuts development time and expense while providing a dependable substitute for traditional techniques. (Ajdarić et al., 2021; Shingare, 2026; Evers, Clénet, and Pfeiffer-Marek, 2022).

## 9.4 Case Study 4: AI in Process Control and Continuous Manufacturing

Because of its uniformity and efficiency, continuous production is becoming more and more important in today's pharmaceutical businesses. Real-time process control has been made possible by the integration of AI into manufacturing systems.

In this instance, Process Analytical Technology (PAT) tools and AI algorithms were used to monitor and regulate industrial factors like:

- The pace of mixing.
- The temperature.
- The rate of flow to ensure ideal conditions, the system continuously evaluated data and modified parameters.



### **Key Outcomes:**

- Enhanced quality and consistency of the product .
- A decrease in batch failures.
- Increased productivity.

Importance:  
This example demonstrates how AI is helping to make pharmaceutical production a more intelligent and automated process.

Overall Takeaways from Case Studies:

Together, the case studies show that AI:

- Lessens the workload associated with experiments .
- Increases the accuracy of predictions .Quickens the development of formulations .
- Enhances the consistency and quality of the product .

These practical uses confirm the increasing significance of AI in the creation of pharmaceutical formulations (Gunjal, 2025; Sartaj et al., 2025).

## **10. Artificial Intelligence's Benefits for Pharmaceutical Formulation Development**

There are many benefits to using artificial intelligence in pharmaceutical formulation creation, including increased productivity, precision, and creativity.

### **10.1 Shorter Development Time**

AI shortens the time needed for formulation development by enabling quick screening and evaluation of several formulation factors. Outcomes can be simulated using predictive models without requiring a lot of laboratory testing.

### **10.2 Economy of Cost**

AI lowers total development costs by lowering experimental trials and resource utilization. This is especially useful for intricate compositions that call for pricey materials.

### **10.3 Increased Predictive Precision**

Large datasets can be analyzed by AI models, which can then find intricate correlations between factors to produce extremely precise forecasts of formulation outcomes like stability and drug release.

### **10.4 Decrease in Workload for Experiments**

Repeated experiments are a part of traditional formulation development. By forecasting ideal circumstances, AI lessens this strain and frees up researchers to concentrate solely on validation investigations.

### **10.5 Better Decision-Making**

Better decision-making during formulation design and optimization is made possible by AI's data-driven insights.

### **10.6 Capacity to Manage Complicated Systems**

AI can model multivariate and nonlinear systems, which are challenging to examine with traditional techniques.

### **10.7 Assistance with Cutting-Edge Drug Delivery Systems**

AI makes it easier to create and optimize intricate drug delivery systems including targeted delivery platforms, liposomes, and nanoparticles.(Prusty and Panda, 2024; Shen et al., 2025; Vengateswaran et al., 2025; Mintaş and Sevimli-Gür, 2024).

## **11. AI's Limitations and Difficulties**

The application of AI in pharmaceutical formulation development faces a number of obstacles despite its many benefits.

### **11.1 Data Quality and Availability**

For training, AI models need vast, high-quality datasets. Model performance may be impacted by pharmaceutical data's frequent limitations, incompleteness, or lack of standardization.

### **11.2 Models' Black-Box Character**



Many AI models are opaque and difficult to understand, particularly deep learning algorithms. This makes it challenging to comprehend how forecasts are produced, which can be problematic in crucial applications.

### 11.3 Excessive Computational

Needs Deep learning in particular necessitates substantial infrastructure and computational resources, which might not be easily accessible in many research environments.

### 11.4 Integration with Current Systems

It can be difficult to integrate AI into conventional pharmaceutical workflows since it calls for adjustments to infrastructure, training, and procedures.

### 11.5 Regulatory Obstacles

Pharmaceutical processes must be transparent and clearly validated, according to regulatory bodies. Regulatory approval of AI-based systems is hampered by the absence of clear norms.

### 11.6 Risk of Overfitting

If AI models are not adequately tested, they may perform well on training data but fail to generalize to new data. Predictions may become erroneous as a result. (Somara et al., 2025; Salunke<sup>7</sup>, 2026; Tade et al., 2023).

## 12. Regulatory and Ethical Issues

To ensure safe and efficient application, a number of ethical and legal issues are raised by the use of AI in pharmaceutical formulation.

### 12.1 Validation and Reliability of the Model

To guarantee that AI models' predictions are precise and repeatable, they must undergo extensive validation. Obtaining regulatory permission requires validation.

### 12.2 Explainability and Transparency

Decision-making procedures must be transparent, according to regulatory agencies. Explainable AI (XAI) models that offer insights into prediction processes are being developed.

### 12.3 Security and Privacy of Data

To maintain confidentiality and adherence to data protection laws, pharmaceutical data—particularly patient-related data—must be safeguarded.

### 12.4 Frameworks for Regulation

Clear regulatory criteria must be developed for the deployment of AI in pharmaceuticals in order to guarantee its safe and uniform application.

Summary:

Even though AI has several benefits for developing pharmaceutical formulations, its successful application depends on resolving its issues. Developing legal frameworks, enhancing model interpretability, and guaranteeing data quality are essential stages toward broad adoption. (Sartaj et al., 2025; Kiruthiga et al., 2025; Salunke<sup>7</sup>, 2026).

## 13. AI's Prospects for Pharmaceutical Formulation Development

It is anticipated that artificial intelligence will revolutionize the development of pharmaceutical formulations in the future. AI is expected to play a significant role in pharmaceutical research and business due to ongoing developments in computational technology, data accessibility, and algorithm design.

### 13.1 AI-Powered Customized Healthcare

Personalized medicine is one of the most promising uses of AI. AI can create personalized medication formulations by analyzing patient-specific data, including age, metabolism, disease state, and genetic profile. This strategy reduces side effects and enhances treatment results.



### 13.2 Combining 3D Printing Technologies

Formulation development is predicted to undergo a revolution when AI and 3D printing are combined. While 3D printing makes it possible to create personalized dosage forms with accurate medication release patterns, AI can optimize formulation parameters.

### 13.3 Self-Optimizing System Development

AI-driven systems that can autonomously design, test, and optimize formulations may be used in pharmaceutical laboratories in the future. These "self-driving laboratories" will speed up medication research and drastically cut down on human meddling.

### 13.4 Technology of Digital Twins

Virtual models that mimic actual systems are called "digital twins." AI-based digital twins can mimic formulation procedures and forecast results in pharmaceutical formulation, improving optimization and risk assessment.

### 13.5 Cloud Computing and Big Data Integration

The scalability and accessibility of AI models will be improved through the use of big data analytics and cloud-based platforms. This will enable academics to work together across geographical boundaries and process massive datasets effectively.

### 13.6 Automation and Continuous Production

By facilitating real-time monitoring, predictive maintenance, and automated process control, artificial intelligence (AI) will significantly contribute to the advancement of continuous manufacturing, improving productivity and product quality.(Kumar and Shahin, 2025; Rajesh and Elumalai, 2025; Rasala4, 2025; Weng et al., 2024).

## 14. Analysis of Gaps

There are still a number of holes in the use of AI in the creation of pharmaceutical formulations, despite tremendous progress.

### 14.1 Insufficient Standardized Datasets

The lack of publicly accessible, consistent datasets for AI model training is one of the main drawbacks. This limits the creation and verification of reliable models.

### 14.2 Limited Application in the Real World

The majority of AI applications in formulation development are still in the research phase. More real-world application and industrial-scale validation are required.

### 14.3 Inadequate Regulations

The creation of comprehensive and unambiguous regulatory frameworks for AI-based pharmaceutical systems is still ongoing. Adoption of AI technologies becomes questionable as a result.

### 14.4 The Requirement for Multidisciplinary Knowledge

Pharmaceutical scientists, data scientists, and engineers must work together for AI to be implemented successfully. Progress may be hampered by a lack of transdisciplinary competence.

### 14.5 Problems with Model Interpretability

Many AI models are difficult to adopt due to their opaque character, especially in regulatory settings where openness is crucial.(Anand, 2025; Somara et al., 2025; Khan et al., 2024)

## CONCLUSION

Pharmaceutical formulation creation is being revolutionized by artificial intelligence through the introduction of data-driven, efficient, and predictive methods. It improves accuracy and formulation quality while drastically cutting



development time, expense, and experimental workload.

AI's enormous potential to revolutionize pharmaceutical sciences is demonstrated by its applications in fields like formulation optimization, drug release prediction, stability research, and sophisticated drug delivery systems. Its influence is further increased by its integration with cutting-edge technologies like digital twins, 3D printing, and continuous manufacturing.

However, to guarantee successful deployment, issues with data accessibility, model interpretability, and regulatory approval must be resolved. The broad use of AI in pharmaceutical formulation will require ongoing research, the creation of standardized datasets, and the creation of regulatory frameworks. In conclusion, artificial intelligence (AI) is a potent and promising instrument that will influence pharmaceutical formulation creation in the future by facilitating quicker, more effective, and creative drug development procedures. (Sartaj et al., 2025; Ali et al., 2024)

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