Role of AI in Drug Formulation

Ms. Apeksha. V. Harpal, Mr. Aryan Dabade, Gauri Mhatre, Dr. Ashish Pagariya, Ms. Anagha Samant

Bhartiya education institute of pharmacy, Nagothane

Abstract

This review presents a critically rewritten and analytically structured discussion on the role of Artificial Intelligence (AI) in drug formulation development. Artificial Intelligence (AI) is transforming drug formulation by improving efficiency, accuracy, and quality in pharmaceutical development. AI technologies including Machine Learning (ML), Artificial Neural Networks (ANN), Deep Learning (DL), Genetic Algorithms (GA), and predictive analytics are transforming traditional pharmaceutical development approaches. Despite its advantages, AI in drug formulation faces several challenges, including data limitations, high implementation costs, regulatory issues, and ethical concerns such as data privacy and transparency. However, the future of AI in drug formulation is promising, with applications in automated manufacturing, predictive modelling, and advanced drug delivery systems. This review highlights AI technologies used in drug formulation, their benefits, limitations, ethical considerations, and future scope in pharmaceutical development.

Keywords

1. Artificial Intelligence
2. Drug Formulation
3. Machine Learning
4. Artificial Neural Network
5. Deep Learning
6. Genetic Algorithms

Abbreviations

1. AI- Artificial Intelligence
2. ML- Machine Learning
3. DL- Deep Learning
4. ANN- Artificial Neural Network
5. RF- Random Forests
6. CQAs-Critical quality attributes
7. SVM-Support Vector Machine
8. DoE- Design of Experiments
9. API -Active Pharmaceutical Ingredient
10. EHRs -Electronic Health Records
11. NLP- Natural Language Processing
12. New chemical Entitity

Introduction

Drug formulation involves designing stable, effective, and safe dosage forms. AI technologies such as machine learning (ML), artificial neural networks (ANN), and deep learning (DL) enable prediction of critical quality attributes (CQAs) and optimization of formulation parameters (Zhang et al., 2024). Artificial Intelligence (AI) has emerged as a powerful tool that can improve drug formulation by analysing large datasets and predicting formulation outcomes. AI technologies such as chatbots and virtual assistants help researchers access formulation information quickly, while Electronic Health Records (EHR) provide patient data that support personalized drug formulations. Automation and robotics improve precision and efficiency in pharmaceutical manufacturing.

Drug formulation traditionally relies on experimental optimization techniques. AI enables predictive modeling that reduces time and cost (Wang et al., 2020). Neural network models demonstrate higher predictive accuracy compared to classical regression approaches (Agatonovic-Kustrin & Beresford, 2000). Traditionally, drug formulation development has relied heavily on empirical methods and trial-and-error experimentation. Researchers conduct multiple laboratory experiments to determine optimal combinations of polymers, binders, lubricants, disintegrants, and other excipients. While this approach has been successful historically, it is time-consuming, resource-intensive, and often inefficient when dealing with complex multi-variable systems. Moreover, modern pharmaceutical products—such as controlled-release systems, nanoparticles, and personalized dosage forms—require precise optimization that exceeds the capability of conventional statistical tools. AI algorithms can help in identifying the most suitable excipients, the optimal dose, and the right drug delivery systems for each formulation.

AI techniques such as machine learning and predictive modelling allow scientists to predict drug–excipient interactions, stability, and bioavailability, reducing the need for extensive laboratory experiments. These technologies help improve product quality and accelerate drug development. However, the use of AI in drug formulation also presents challenges, including data quality issues, high costs, regulatory requirements, and ethical concerns. This review discusses the role of AI technologies in drug formulation, along with their benefits, limitations, ethical considerations, and future scope in pharmaceutical sciences.

AI in Drug Formulation

1. Machine Learning (ML): The Engine of Predictive Analytics

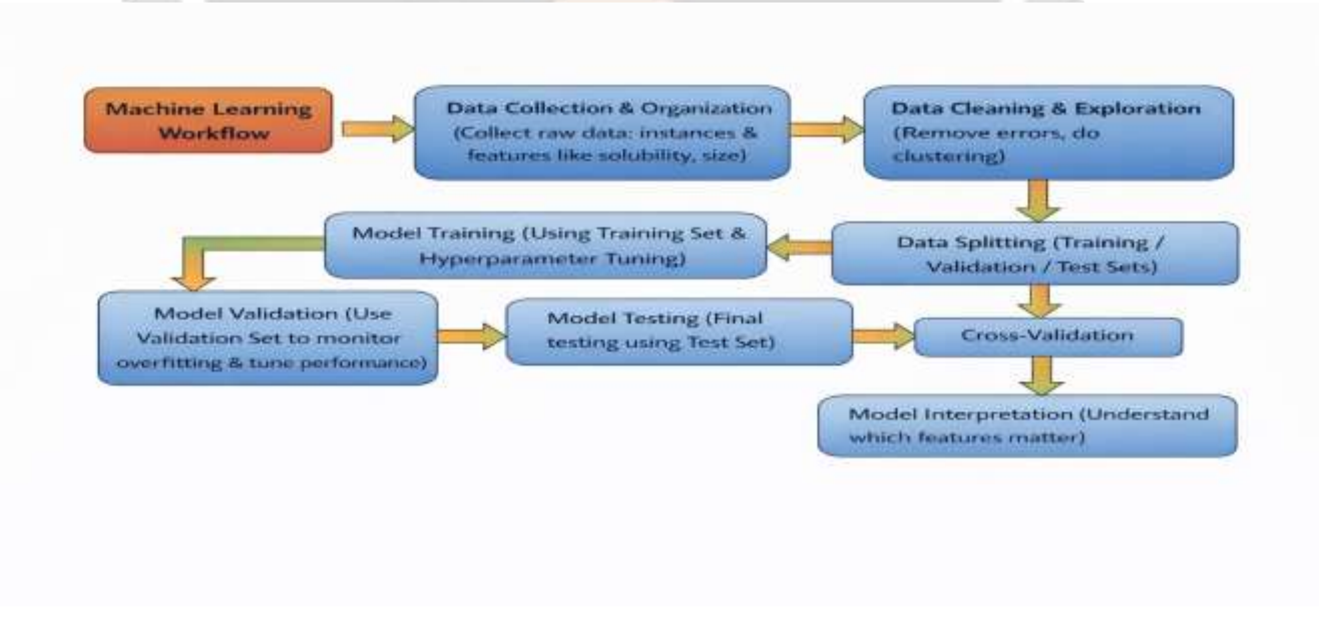
Machine Learning serves as the foundational pillar of AI in the pharmaceutical sector. By utilizing algorithms that "learn" from experimental data rather than following rigid, pre-defined rules, ML can identify complex patterns that govern drug behaviour.

Physicochemical Predictions: ML models, such as Random Forests (RF) and Support Vector Machines (SVM), are highly effective at predicting drug solubility and dissolution rates. These are critical parameters, as nearly 40% of new chemical entities are poorly water-soluble.

Stability & Bioavailability: Beyond initial design, ML helps forecast the long-term stability of a compound by simulating degradation pathways. It also predicts bioavailability the proportion of a drug that enters the circulation by modelling the interaction between the drug's molecular descriptors and biological barriers.

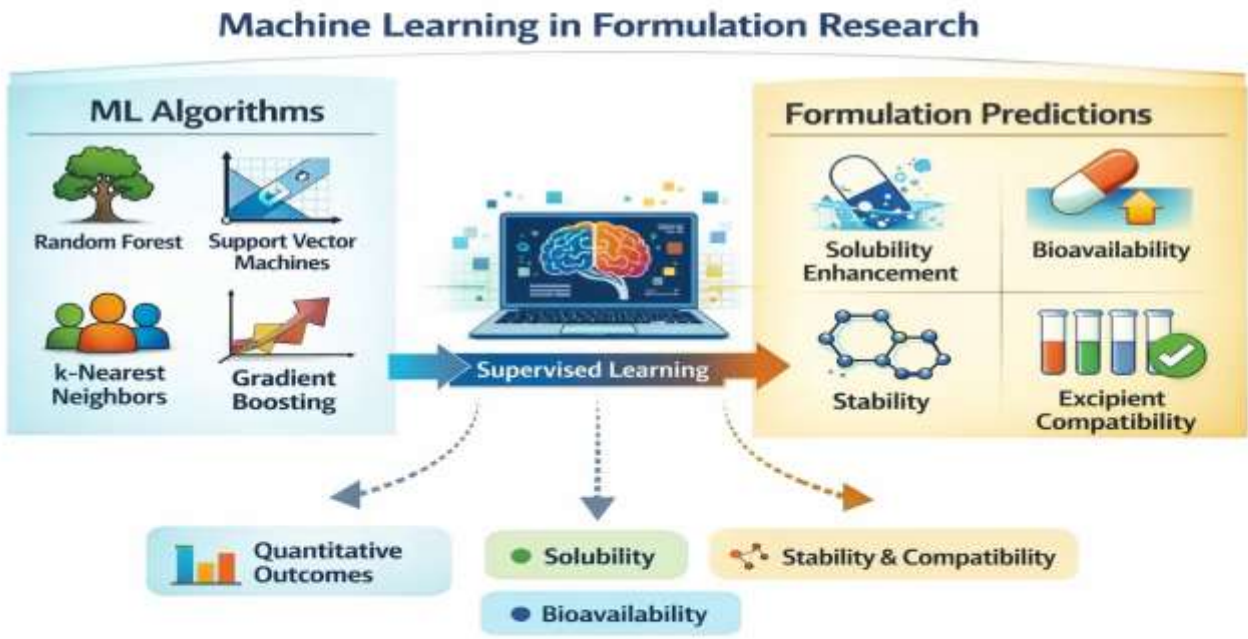
ML models excel when they are trained on large, detailed datasets. In the world of pharmaceutical development, these datasets might include information about a drug’s properties, excipients, manufacturing techniques, and performance expectations. Once trained, the ML model can spot patterns that aren’t obvious to the human eye, helping scientists make more accurate decisions early in the development process.

Machine Learning Workflow in Drug Formulation



There are two categories of ML :-

1. Supervised learning
2. Unsupervised learning



2. Deep Learning (DL): Mastering Complexity

Deep learning represents an advanced extension of neural networks with multiple hidden layers. These models are capable of managing highly nonlinear pharmaceutical datasets. Applications include nanoparticle size optimization, drug loading efficiency prediction, and image-based defect detection in tablet manufacturing.

As a specialized subset of ML, Deep Learning utilizes multi-layered architectures to process vast amounts of unstructured data. Its primary strength lies in its ability to perform "automatic feature extraction," removing the need for scientists to manually input every variable.

Advanced Image Analysis: DL is revolutionary in quality control, specifically through Convolutional Neural Networks

Criteria	Supervised Learning	Unsupervised Learning
Definition	Learns from labelled data each input has a known output	Works with unlabelled data finds hidden patterns without predefined answers
Human Involvement	High. requires data labelling before training	Low. can work directly with raw, unstructured data
Purpose	Used for prediction and classification tasks	Used for pattern recognition, grouping, and data exploration
Example Use in Pharma	Predicting tablet quality based on excipient type and manufacturing conditions	Grouping formulations based on disintegration behaviour or physicochemical traits
Algorithms Examples	Linear regression, logistic regression, decision trees, random forest, support vector machines, deep learning models	K-means clustering, hierarchical clustering, principal component analysis (PCA), self-organizing maps (SOM)
Performance Focus	High accuracy in predicting specific outcomes	Good for discovering trends or organizing large data sets

(CNNs). These are used for high-speed microscopy and identifying minute tablet defects (e.g., capping or lamination) that the human eye might miss.

Molecular Mapping: DL models can analyse molecular structures to predict how a new drug might bind to a target protein, significantly narrowing the field of potential candidates during the early formulation stage.

Applications of Deep Learning in Drug Formulation

1. Image-Based Granule Morphology Analysis Convolutional Neural Networks (CNNs) analysis microscopic images to evaluate particle shape and size.

2. Tablet Surface Defect Detection Detects cracks, coating defects, and surface irregularities in tablets.
3. Spectroscopic Data Interpretation Interprets NIR and Raman spectroscopy data for real-time quality monitoring
4. Real-Time Manufacturing Monitoring

3. Artificial Neural Networks (ANN): Mimicking Biological Logic

ANN models simulate biological neurons and are widely applied in tablet optimization (Takayama et al., 2000). ANN-based models achieve predictive accuracy above 90% in dissolution studies (Singh et al., 2021).

ANNs are designed to replicate the signal-processing capabilities of the human brain, consisting of interconnected "neurons" that weight different inputs to produce an output. In pharmaceutical science, they are particularly valued for their ability to handle non-linear relationships.

Release Pattern Optimization: ANNs are used to design sustained-release dosage forms. By adjusting variables like polymer concentration and coating thickness, the network can predict the exact drug release profile over 12 to 24 hours.

Excipient Synergy: Selecting the right combination of inactive ingredients (excipients) is often a "trial-and-error" process. ANNs can optimize these concentrations to ensure the final product is both stable and effective, reducing the number of physical laboratory batches required by up to 70%.

AI Techniques Used in Pharmaceutical Formulation Development

Technique	Description	Applications in drug Formulation	Benefits
Machine Learning (ML)	A subset of AI that uses algorithms to identify patterns in data.	Optimization of excipient selection, predicting drug release rates, and formulation stability.	Reduces formulation development time and costs.
Deep Learning (DL)	A type of ML using neural networks with many layers to learn from data.	Predicting drug interactions, stability testing, and bioavailability optimization.	Provides accurate predictions for complex formulation designs.
Natural Language Processing (NLP)	A technique for analyzing and interpreting human language.	Analyzing scientific literature for new formulation techniques, identifying trends in excipient use.	Speeds up research and decision-making processes.
Predictive Analytics	Uses historical data to predict future outcomes.	Anticipating drug stability, patient response, and formulation success.	Improves The likelihood of formulation success.

Traditional Drug Formulation vs. AI-Based Formulation

The evolution of pharmaceutical science is best understood by comparing the legacy "Trial-and-Error" framework with the emerging "Digital Twin" or AI-driven paradigm. While the traditional approach has been the industry standard for over a century, its inherent limitations are increasingly at odds with the modern need for rapid, cost-effective drug delivery.

Comparative Summary Table

Criteria	Traditional Formulation Techniques	AI-Based Formulation Optimization
Approach	Depends heavily on hands-on experiments and a trial-and-error approach.	Utilizes advanced computational tools and data-driven models to predict and optimize formulations.

Time Efficiency	Requires longer development time due to repeated manual experiments	Reduces development time by simulating results and minimizing unnecessary experiments
Cost Effectiveness	Often costly due to wasted materials, prolonged testing, and high labour needs	Helps lower costs by reducing failed trials and limiting the use of resources
Data Utilization	Makes minimal use of existing data and lacks real-time input integration	Leverages large, varied datasets both historical and real-time to make informed decisions.
Predictive Reliability	Susceptible to inconsistencies and human error in predictions.	Offers accurate and consistent predictions, enabling better control over formulation variables.
Scalability	Scaling up production is often limited by manual processes.	Easily scalable with the help of automation and intelligent systems.
Innovation Capability	Creativity is mostly driven by human experience and intuition.	Encourages discovery of innovative drug combinations and delivery methods through AI insights.
Regulatory Alignment	Follows traditional regulatory pathways but adopts changes slowly.	Faces regulatory challenges due to complex AI models, which require transparency and explanation.
Common Challenges	Requires extensive manpower, time, and expert knowledge.	Relies on high-quality data and needs clear understanding of AI decision-making processes.

Applications of AI in Drug Formulation

The transition to AI-driven formulation is not a singular event but a series of targeted integrations across the development lifecycle. From the molecular level to the final patient dose, AI acts as a precision tool for optimization.

1.Pre-formulation Studies: Predictive Physical Chemistry

Pre-formulation is the first window into a drug's potential. Traditionally, determining the fundamental physical and chemical properties of a New Chemical Entity (NCE) required months of laboratory assays.

2. Excipient Compatibility: Preventing Chemical Conflict

AI systems can suggest suitable excipient combinations that enhance drug performance and stability using historical formulation datasets combined with cheminformatics and material property databases. For instance, supervised learning models (random forest, gradient boosting, deep neural networks) can classify excipients based on predicted com patibility with APIs. In contrast, models based on regression can predict ideal excipient ratios to achieve target dissolution, compressibility, or disintegration times

3. Optimization of Dosage Forms: The Search for the "Golden Formula"

Whether designing a simple tablet or a complex suspension, the ratio of ingredients is critical. AI driven **Design of Experiments (DoE)** has replaced traditional manual scaling.
Dynamic Geometries: For **controlled-release formulations**, ML algorithms determine the exact polymer concentration and surface area needed to achieve a specific release curve.

Process Efficiency: AI optimizes the manufacturing parameters—such as compression force for tablets or stirring speed for suspensions—ensuring that every batch meets the highest quality standards.

4. Stability Studies: Compressing Time

Stability testing is one of the longest phases of drug development, often requiring 6 to 24 months of "real-time" data to satisfy regulators.

Accelerated Forecasting: AI algorithms analyze short-term, high-stress data (e.g., extreme heat and humidity) to predict **long-term shelf life** and **degradation rates**.

Market Readiness: This allows pharmaceutical companies to file for regulatory approval with a higher degree of confidence in their product's longevity, effectively accelerating the global product launch.

5. Personalized Medicine: The Patient-Centric Future

Personalized medicine is a growing trend in the pharmaceutical industry, and AI plays a critical role in formulating drugs for specific patient populations. AI can analyze genetic, environmental, and lifestyle data to predict how an individual might respond to a drug. Personalized formulations tailored to these predictions can lead to more effective and safer treatments.

6. AI in 3D-Printed Dosage Forms

Artificial Intelligence (AI) is revolutionizing 3D printed drug formulations by enabling personalized and efficient medicine production. AI helps design patient-specific dosage forms by analysing individual factors like age and health conditions. It optimizes drug release, dosage strength, and tablet shape, improving both safety and effectiveness.

AI also streamlines the 3D-printing process by adjusting key factors like print speed and temperature. In studies, AI models such as Artificial Neural Networks (ANNs) have successfully predicted how tablet structure impacts drug release. This leads to better control, faster development, and consistent quality.

AI Technology used in Drug Formulation

Artificial Intelligence (AI) technologies such as chatbots and virtual assistants, Electronic Health Records (EHR), and automation and robotics are increasingly used in drug formulation to improve efficiency, accuracy, and product quality. AI helps researchers design better formulations by analyzing large datasets and predicting drug properties such as stability, dissolution, and bioavailability (Paul et al., 2021; Patel et al., 2023).

AI-based chatbots and virtual assistants use natural language processing (NLP) to help researchers quickly access scientific literature, formulation guidelines, and excipient compatibility data. These tools assist scientists in selecting suitable excipients and optimizing formulation parameters, which reduces development time and improves decision-making (Jiang et al., 2017; Patel et al., 2023). Chatbots can also support pharmaceutical research by providing instant access to formulation databases and drug information.

Electronic Health Records (EHR) store patient information such as age, weight, disease condition, allergies, and medication history. AI can analyze EHR data to support personalized drug formulation and individualized dosage design, improving therapeutic outcomes and reducing adverse drug reactions (Jiang et al., 2017; Yu, 2008). The use of EHR data enables pharmaceutical scientists to develop safer and more effective formulations tailored to patient needs.

Automation and robotics play an important role in drug formulation by performing tasks such as weighing, mixing, granulation, coating, and tablet compression with high precision. Robotic systems allow high-throughput screening of multiple formulations at the same time, which accelerates drug development and improves reproducibility (Basavaraj et al., 2022; Rathore & Winkle, 2009). Automation also reduces human error and ensures consistent product quality during formulation and manufacturing.

In addition, AI techniques such as machine learning help predict drug–excipient interactions, drug stability, and bioavailability. These predictions reduce the traditional trial-and-error approach and lower the cost and time required for formulation development (Paul et al., 2021; Patel et al., 2023). AI also supports the development of controlled-release formulations and advanced drug delivery systems by identifying optimal formulation conditions.

Overall, AI technologies including chatbots, EHR, and automation and robotics are transforming drug formulation by making the process faster, more accurate, and cost-effective. In the future, AI is expected to further improve pharmaceutical formulation and enable the development of personalized medicines.

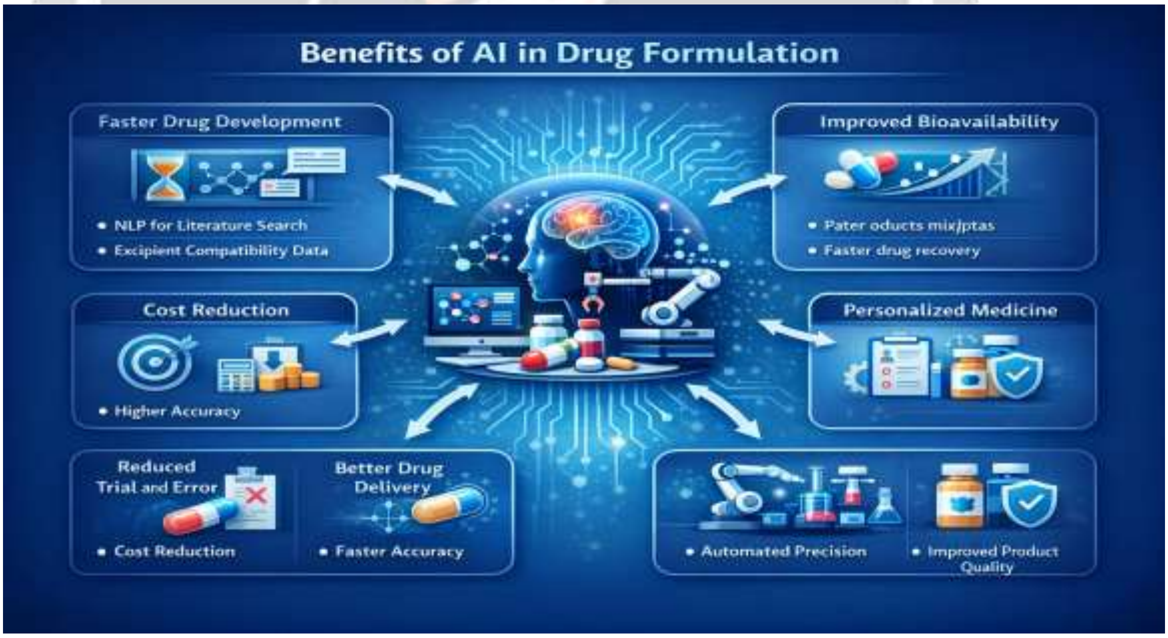
Benefits of AI in Drug Formation

Artificial Intelligence (AI) has become an important tool in drug formulation because it improves efficiency, accuracy, and quality in pharmaceutical development. AI techniques such as machine learning and data analytics help scientists design optimized formulations by analyzing large datasets and predicting drug properties. One major benefit of AI in drug formulation is the reduction in development time. Traditional formulation methods rely on trial-and-error experiments, but AI can predict suitable excipients, drug–excipient compatibility, and optimal formulation conditions, which accelerates the development process (Paul et al., 2021; Patel et al., 2023).

AI also improves the accuracy and quality of drug formulations. Machine learning models can predict important parameters such as solubility, stability, dissolution rate, and bioavailability, leading to more effective and stable pharmaceutical products (Yu, 2008; Rathore & Winkle, 2009). This reduces formulation failures and ensures consistent product quality. Another important benefit is cost reduction. By minimizing experimental trials and reducing material wastage, AI helps pharmaceutical industries lower research and production costs (Basavaraj et al., 2022).

AI supports personalized medicine by analyzing patient data and helping design drug formulations tailored to individual needs. This improves therapeutic effectiveness and reduces adverse drug reactions (Jiang et al., 2017). AI also enhances automation in pharmaceutical manufacturing, where robotic systems perform formulation processes such as mixing, granulation, and tablet compression with high precision and minimal human error (Basavaraj et al., 2022).

Furthermore, AI improves decision-making by providing data-driven insights during formulation development. It helps researchers select the best formulation strategies and optimize drug delivery systems such as controlled-release and targeted delivery formulations (Patel et al., 2023). Overall, AI plays a vital role in modern drug formulation by making the process faster, more accurate, cost-effective, and reliable. In the future, AI is expected to further transform pharmaceutical formulation and enable the development of advanced and personalized medicines.



Limitations and challenges of AI in Drug formulation

Artificial Intelligence (AI) has significantly improved drug formulation; however, several limitations and challenges still affect its implementation in pharmaceutical development. One major challenge is the availability and quality of data. AI models require large and high-quality datasets to make accurate predictions, but pharmaceutical data are often limited, incomplete, or inconsistent. Poor-quality data can lead to incorrect predictions and unreliable formulations (Paul et al., 2021; Patel et al., 2023).

Another important limitation is the high cost of implementation. The use of AI technologies requires advanced software, specialized equipment, and skilled professionals, which can be expensive for small pharmaceutical companies and research laboratories (Basavaraj et al., 2022). In addition, maintaining AI systems and updating databases requires continuous investment.

AI models also face challenges related to interpretability and transparency. Many AI algorithms function as "black boxes," meaning it is difficult to understand how the model arrives at a particular formulation decision. This lack of transparency can reduce trust and make regulatory approval more difficult (Rathore & Winkle, 2009). To provide transparency, techniques such as explainable AI (XAI), including SHAP (Shapley Additive Explanations) and LIME (Local Interpretable Model-Agnostic Explanations), are currently being explored [37] However, one of the ongoing challenges is balancing predictive accuracy with interpretability because, without clear justifications, AI recommendations may be disregarded in clinical or regulatory decision-making[38]

Regulatory and legal issues are another challenge in applying AI to drug formulation. In 2022, the European Medicines Agency (EMA) formally qualified Unlearn's AI driven approach for running smaller, more efficient clinical trials.[33] In the case of FDA, there is no well-documented case (publicly verifiable) where an AI model for formulation or dosage was fully accepted in a drug application submission as a core decision-making model [34] Pharmaceutical products must meet strict regulatory standards, and the use of AI in formulation development requires validation and documentation to ensure safety and effectiveness. Regulatory guidelines for AI-based drug formulation are still evolving, which can slow down implementation (Yu, 2008).

Another limitation is the lack of skilled professionals trained in both pharmaceutical sciences and artificial intelligence. Effective use of AI requires knowledge of programming, data analysis, and pharmaceutical formulation, which may not always be available (Jiang et al., 2017).

AI systems also depend heavily on technology and infrastructure. Technical issues such as software errors, system failures, or cybersecurity risks can disrupt formulation processes and compromise data security (Paul et al., 2021).

AI models require a significant amount of data for accurate predictions. However, in some cases, there may be limited data available for a particular drug or population, leading to less accurate predictions or biased results. For instance, rare diseases may have limited data available, which can be a significant challenge for developing AI models. Additionally, the data used to train AI models may not be representative of the population of interest, which can lead to biased results. Moreover, some types of data, such as longitudinal data or real-world evidence, may not be readily available, which can limit the utility of AI models. These limitations highlight the need for the careful consideration of the quality and representativeness of the data used to develop AI models.

AI models are generally trained on large datasets, which can be biased toward the average responses observed in the data. As a result, the models may not be able to accurately predict drug responses for individuals who deviate significantly from the average response. This is particularly concerning for drugs that have a wide range of responses in different patients (such as in cancer), where the variability can be significant[40]

Overall, although AI offers many advantages in drug formulation, challenges such as data limitations, high costs, regulatory issues, lack of expertise, and technical constraints must be addressed to fully utilize its potential in pharmaceutical development.

Ethical and Legal Considerations AI in drug formulation

The use of Artificial Intelligence (AI) in drug formulation offers many advantages, but it also raises important ethical and legal considerations. These issues must be addressed to ensure safe, effective, and responsible use of AI in pharmaceutical development. Ethical and legal challenges include data privacy, data security, transparency, accountability, and regulatory compliance. Addressing these concerns is essential for maintaining patient trust and ensuring that AI-based drug formulations meet required safety standards (Jiang et al., 2017; Paul et al., 2021).

One major concern is patient privacy, as sensitive health data are often used to train AI models. Data safety and security represent crucial parameters that demand significant attention and cannot be overlooked. It is important to ensure that patient data are collected and used in a way that protects their privacy and respects their rights. Data ownership is another ethical concern when using AI in drug development. In some cases, data may be collected from patients without their explicit consent, and it may not be clear who owns the data or who has the right to use it. This can lead to conflicts between patients, researchers, and pharmaceutical companies. 7,41,42]

Regulatory agencies are tasked with the development of stringent protocols, guidelines, and standardized evaluation processes to effectively integrate AI into drug development. These measures should encompass multiple dimensions, including the ethical considerations of animal welfare and patient safety. Animal testing, which plays a pivotal role in drug development, necessitates a commitment to reducing, refining, and replacing animal models whenever feasible, aligning with ethical principles. Prioritizing patient safety, AI models must undergo thorough validation and testing to ensure their reliability and accuracy. An important step in addressing the regulatory and ethical implications of AI in drug development is the release of the discussion paper by the U.S. Food and Drug Administration (FDA) entitled, "Using Artificial Intelligence & Machine Learning in the Development of Drug and Biological Products." This document provides an overview of the role of AI in drug discovery, nonclinical research, and clinical research. Additionally, it outlines recommended practices for the application of AI and machine learning. This FDA initiative marks an important milestone in regulating the use of AI in healthcare and paves the way for new opportunities in the sector. It signifies the recognition of the potential benefits and challenges associated with AI in drug development and sets the stage for future regulatory advancements in this domain [43]

Another legal issue is accountability and liability. If an AI-designed formulation causes harm, it may be difficult to determine who is responsible, such as the software developer, pharmaceutical company, or researcher. Clear legal guidelines are needed to define responsibility and ensure patient safety (Paul et al., 2021).

Bias and fairness are also ethical concerns in AI-based drug formulation. If AI systems are trained on limited or biased datasets, they may produce inaccurate or unfair results, which can affect drug effectiveness and safety for certain populations (Jiang et al., 2017).

Overall, ethical and legal considerations play a crucial role in the application of AI in drug formulation. Proper data protection, transparency, regulatory compliance, and accountability are necessary to ensure the safe and responsible use of AI in pharmaceutical development. Addressing these challenges will help maximize the benefits of AI while minimizing risks in drug formulation.

Future Scope of AI in Drug Formation

The future of pharmaceutical research is undergoing a transformation thanks to rapid advances in Artificial Intelligence (AI) and Machine Learning (ML). As technology continues to evolve, sophisticated deep learning methods such as convolutional neural networks (CNNs) and recurrent neural networks (RNNs) are playing an increasingly important role. These tools are capable of handling large and complex datasets, making it possible to deliver more accurate predictions about how drugs behave and what outcomes they may produce in patients.

AI might revolutionize the pharmaceutical industry in the future to accelerate drug discovery and drug development. Virtual screening techniques will rapidly analyse enormous chemical libraries and find therapeutic candidates with required features, accelerating lead compound identification.AI-powered monitoring systems will allow remote patient care and medication adherence. Wearable gadgets and sensors will continuously gather data for AI algorithms to propose personalized therapy and better compliance. AI improves clinical trial design, patient selection, and recruitment. AI algorithms will use electronic health records, biomarkers, and genetic profiles to find appropriate patients, lower trial costs, and speed up approval. AI-enabled precise medicine could categorize patients, predict therapy responses, and customize medicines by analyzing genomes, proteomes, and clinical records.

The future of AI in pharmacy holds exciting possibilities, particularly in the realm of real-time healthcare monitoring. AI-powered wearable devices and sensors could continuously monitor patients' vital signs and drug responses, providing real-time data that could inform treatment decisions.

The use of artificial intelligence in various segments of healthcare is growing daily, from the triage and screening of clinical risk prediction to diagnosis [44] Clinical applications of AI have the potential to increase diagnosis accuracy and healthcare efficiency.

AI's ability to analyze genomic data quickly makes it an ideal tool for accelerating vaccine development. AI models can be used to predict viral mutations, identify potential vaccine candidates, and optimize clinical trial designs.

Another important future scope is the integration of AI with automation and robotics in pharmaceutical manufacturing. Fully automated systems may be able to design, test, and produce drug formulations with minimal human intervention. This will improve precision, reduce human error, and increase production efficiency (Basavaraj et al., 2022). AI-driven robots can also perform high-throughput screening of formulations, enabling faster identification of optimal formulations.

AI is also expected to improve predictive modeling and simulation in drug formulation. Advanced AI models will be able to simulate formulation processes and predict the performance of dosage forms before actual manufacturing, saving time and resources (Rathore & Winkle, 2009). In addition, AI will support quality control and quality assurance by detecting formulation defects and ensuring consistent product quality.

In the future, AI may enable the creation of self-optimizing formulations, where AI systems continuously analyze data and adjust formulation parameters to achieve the best results. Cloud computing and big data technologies will further enhance AI capabilities by allowing access to large pharmaceutical datasets and real-time analysis (Paul et al., 2021).

Looking ahead, the future scope of AI in drug formulation is very promising. AI is expected to transform pharmaceutical formulation by enabling faster drug development, personalized medicines, automated manufacturing, and improved drug delivery systems. Continued advancements in AI technology will further enhance its role in pharmaceutical sciences and drug formulation.

Conclusion

Artificial Intelligence has become an important tool in drug formulation by improving efficiency, accuracy, and product quality. AI technologies such as chatbots, Electronic Health Records, and automation and robotics help optimize formulation processes and reduce development time. AI also supports personalized medicine and advanced drug delivery systems by analyzing large datasets and predicting formulation outcomes.

Despite these advantages, AI in drug formulation faces challenges such as data limitations, high costs, regulatory issues, and ethical concerns. Addressing these challenges is necessary for the successful implementation of AI in pharmaceutical development. The future of AI in drug formulation is promising, with potential applications in automated formulation design, predictive modeling, and personalized medicine. Continued advancements in AI technology will further enhance drug formulation and improve healthcare outcomes.

References

1. Paul, D., Sanap, G., Shenoy, S., et al. (2021). Artificial Intelligence in Drug Discovery and Development. Drug Discovery Today, 26(1), 80–93.
2. Renuka G Pawar, Mr. Vilas A. Arsul, Mr. Prakash V. Maske ISSN (Online) 2581-9429.
3. Joshi, S., & Sheth, S. (2025). Artificial Intelligence (AI) in Pharmaceutical Formulation and Dosage Calculations. Pharmaceutics, 17(11), 1440.
4. Agarwal, B., Gaware, S., More, N., et al. (2026). A Review Exploring the Translational Perspective of Artificial Intelligence in Drug Discovery and Formulation Development. Annales Pharmaceutiques Françaises.
5. yadav, A., Singh, G., Singh, M., & Chaudhary, A. (2025). Artificial Intelligence in Optimizing Formulations and Excipients: Revolutionizing Pharmaceutical Product Development. Journal of Advanced Scientific Research.
6. Dey, H., Arya, N., Mathur, H., Chatterjee, N., & Jadon, R. (n.d.). Exploring the role of artificial intelligence and machine learning in pharmaceutical formulation design.
7. Patel L., Shukla T., Huang X., et al. (2020). Applications of Artificial Intelligence in Pharmaceutical Formulation Development. Pharmaceutics, 12(6), 593.
8. Takayama, K., et al. (2000). Application of artificial neural network in formulation development. Journal of Controlled Release, 68(2), 175–186.
9. Agatonovic-Kustrin, S., & Beresford, R. (2000). Basic concepts of artificial neural network modeling and its application in pharmaceutical research. Journal of Pharmaceutical and Biomedical Analysis, 22(5), 717–727.
10. Wang, S., et al. (2020). Machine learning in pharmaceutical development. International Journal of Pharmaceutics, 590, 119980.
11. Anuja Ghaywat, Int. J. of Pharm. Sci., 2025, Vol 3, Issue 10, 1199-1211
12. Alvarado, C., & Perez, F. (2022). Machine learning applications in personalized medicine for pharmacy practice. Pharmaceutical Sciences, 28(1), 22-30.
13. Banerjee, S., &Sen, S. (2020). The role of AI in the formulation and delivery of drugs. Pharmaceutics, 12(6), 1-9.
14. Patel, H., et al. (2023). Artificial Intelligence in Pharmaceutical Formulation Development. Pharmaceutics, 15(3).
15. Schölkopf B., Tsuda K., Vert J.P. MIT Press; 2004. Support vector machine applications in computational biology.
16. Chen H., Engkvist O., Wang Y., Olivecrona M., Blaschke T. The rise of deep learning in drug discovery. Drug Discovery Today. 2018;23(6):1241–1250.
17. Gupta, A., Vaidya, K., & Boehnke, N. (n.d.). AI and machine learning in pharmaceutical formulation and manufacturing of personalized medicines.
18. Zhavoronkov, A., Ivanenkov, Y. A., Aliper, A., et al. (2019). Deep learning enables rapid identification of drug candidates. Nature Biotechnology, 37(9), 1038–1040.
19. Ekins, S. (2016). The next era: Deep learning in pharmaceutical research. Pharmaceutical Research, 33(11), 2594–2603.

20. LeCun, Y., Bengio, Y., & Hinton, G. (2015). Deep learning. Nature, 521(7553), 436–444.
21. Goodfellow, I., Bengio, Y., & Courville, A. (2016). Deep Learning. MIT Press.
22. Liu, R., et al. (2019). Convolutional neural networks for particle size analysis in pharmaceutical powders. *Powder Technology, 360*, 123–132.
23. Wu, H., Khan, M. A., & Hussain, A. (2020). Deep learning-based image analysis for pharmaceutical particle morphology characterization. *International Journal of Pharmaceutics, 583*, 119387.
24. Wang, Z., et al. (2020). Deep learning for automated tablet defect detection in pharmaceutical manufacturing. *Computers in Industry, 121*, 103263.
25. Gao, Y., et al. (2021).CNN-based real-time defect detection system for pharmaceutical tablets. *Journal of Pharmaceutical Innovation, 16*, 467–479.
26. Ning, Y., et al. (2022).Vision-based deep learning framework for coating defect detection in tablets. *Advanced Engineering Informatics, 52*, 101560.
27. Zhang, L., et al. (2022).Real-time pharmaceutical monitoring using NIR spectroscopy and convolutional neural networks. *Sensors, 22*(5), 1876.
28. Basavaraj, S., et al. (2022). Automation and Robotics in Pharmaceutical Industry. International Journal of Pharmaceutical Sciences Review and Research.
29. Yu,L.X.; Amidon, G.; Khan, M.A.; Hoag, S.W.; Polli, J.; Raju, G.K.; Woodcock, J. Understanding pharmaceutical quality by design. Aaps J. 2014, 16, 771–783.
30. Rathore, A. S., & Winkle, H. (2009). Quality by Design for Biopharmaceuticals. Nature Biotechnology, 27(1), 26–34.
31. Topol, E. (2019). High-performance Medicine: The Convergence of Human and Artificial Intelligence. Nature Medicine, 25(1), 44–56.
32. Ribeiro, M.T.; Singh, S.; Guestrin, C. Why should I trust you? : Explaining the predictions of any classifier. In Proceedings of the ACMSIGKDD International Conference on Knowledge Discovery and Data Mining, San Francisco, CA, USA, 13–17 August 2016; pp. 1135–1144
33. European Medicines Agency. Qualification Opinion for PROCOVA™: An AI-Based Approach for Prognostic Covariate Adjustment in Clinical Trials; European Medicines Agency: Amsterdam, The Netherlands, 2022**.**
34. US Food and Administration. Artificial Intelligence and Machine Learning in Drug Development: Guidance for Industry; US Food and Drug Administration: Silver Spring, MD, USA, 2023.
35. Yu, L. X. (2008). Pharmaceutical Quality by Design: Product and Process Development. Pharmaceutical Research, 25(4), 781–791.
36. Jiang, F., Jiang, Y., Zhi, H., et al. (2017). Artificial Intelligence in Healthcare: Past, Present and Future. Stroke and Vascular Neurology, 2(4), 230–243.
37. Lundberg, S.M.; Lee, S.I. A unified approach to interpreting model predictions. Adv. Neural Inf. Process. Syst. 2017, 30, 4765–4774.
38. Holzinger, A.; Biemann, C.; Pattichis, C.S.; Kell, D.B. What do we need to build explainable AI systems for the medical domain? arXiv 2017, arXiv:1712.09923.
39. Sarker, I.H. Machine Learning: Algorithms, Real-World Applications and Research Directions. SN Comput. Sci. 2021, 2, 160.
40. Sarmadi, A.; Hassanzadeganroudsari, M.; Soltani, M. Artificial Intelligence and Machine Learning Applications in Vaccine Development. In Bioinformatics Tools for Pharmaceutical Drug Product Development; Wiley: Hoboken, NJ, USA, 2023; pp. 233–253.
41. Gerke, S.; Minssen, T.; Cohen, G. Ethical and Legal Challenges of Artificial Intelligence-Driven Healthcare. In Artificial Intelligence in Healthcare; Elsevier: Amsterdam, The Netherlands, 2020; pp. 295–336.
42. Naik, N.; Hameed, B.M.Z.; Shetty, D.K.; Swain, D.; Shah, M.; Paul, R.; Aggarwal, K.; Ibrahim, S.; Patil, V.; Smriti, K.; et al. Legal and Ethical Consideration in Artificial Intelligence in Healthcare: Who Takes Responsibility? Front. Surg. 2022, 9, 266.
43. FDA. Using Artificial Intelligence & Machine Learning in the Development of Drug and Biological Products; Food and Drug Administration: Silver Spring, MD, USA, 2023.
44. Pokhriyal, P.; Chavda, V.P.; Pathak, M. Future Prospects and Challenges in the Implementation of AI and ML in Pharma Sector. In Bioinformatics Tools for Pharmaceutical Drug Product Development; Wiley: Hoboken, NJ, USA, 2023; pp. 401–416.
45. Patel H. A Review: Future Aspects of Artificial Intelligence, Big Data, and Robotics in the Pharmaceutical Industry. 2021.