



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



Review Article

AI and Machine Learning in Formulation Development

Anuja Ghaywat*, Ramdas Darade, Vikram Saruk, Manoj Garad, Swati Gaykar, Priti Bhure, Komal Gunjal

Jagadamba Education Society's SND College of Pharmacy, Yeola, Maharashtra, India

ARTICLE INFO

Published: 13 Oct 2025

Keywords:

Artificial intelligence,
Machine learning,
Formulation development,
Drug delivery

DOI:

10.5281/zenodo.17339741

ABSTRACT

Artificial Intelligence (AI) and Machine Learning (ML) are transforming the pharmaceutical industry by introducing data-driven, predictive, and highly personalized approaches to drug formulation and delivery. These technologies are revolutionizing traditional practices by enhancing formulation accuracy, accelerating development timelines, and reducing costs. From solid oral dosage forms and 3D-printed medications to nanomedicine, injectable biologics, and intelligent medical devices, AI applications are enabling more precise, effective, and tailored treatments. This review explores the capabilities of AI and ML in pharmaceutical formulation, highlighting their use in optimizing drug release, predicting stability, and streamlining manufacturing processes. It discusses the integration of neural networks, natural language processing, and computer vision, while also acknowledging current limitations such as data quality, model transparency, and regulatory challenges. Furthermore, it presents case studies from leading pharmaceutical innovators and outlines the future direction of AI/ML technologies in advancing personalized medicine and improving patient outcomes.

INTRODUCTION

The pharmaceutical industry is experiencing a paradigm shift driven by the integration of Artificial Intelligence (AI) and Machine Learning (ML). These transformative technologies, once confined to computer science, are now at the forefront of pharmaceutical formulation and drug delivery. With their ability to analyse vast datasets, recognize patterns, and make predictive decisions,

AI and ML are redefining how medicines are discovered, developed, and personalized. Traditional drug formulation has long relied on trial-and-error experimentation, consuming significant time, cost, and resources. AI offers a powerful alternative one that enables scientists to simulate outcomes, predict formulation behaviour, and rapidly optimize drug combinations. This shift not only accelerates development but also allows

***Corresponding Author:** Anuja Ghaywat

Address: Jagadamba Education Society's SND College of Pharmacy, Yeola, Maharashtra, India

Email ✉: anujaghaywat2004@gmail.com

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.



for the design of personalized therapies tailored to individual patient profiles.

In this review, we explore the diverse applications of AI and ML across pharmaceutical systems, from oral solid dosage forms and nanomedicine to transdermal patches and advanced medical devices. We examine how these tools enhance formulation efficiency, ensure quality control, and support innovation in drug delivery. Additionally, we address the limitations and ethical considerations surrounding AI adoption and outline emerging trends that promise to shape the future of pharmaceutical science.

Artificial Intelligence: A Human-Like Approach to Problem Solving

Artificial Intelligence (AI) refers to the ability of machines to carry out tasks that typically require human intelligence such as understanding language, recognizing patterns, solving problems, and making decisions. At its core, AI combines the principles of computer science with insights into how people think and learn. In simple terms, intelligence involves using reasoning, memory, and experience to reach a goal. AI aims to replicate these abilities in machines, allowing them to think and act in ways that resemble human behaviour often with greater speed and efficiency. As described by early researchers like Poole and Goebel, AI is about designing computers that can act intelligently, much like humans would in similar situations.

Today, Artificial Intelligence and its subset, Machine Learning, are revolutionizing many fields from healthcare to finance to everyday technology. These tools are not just automating tasks but are transforming how we approach problem-solving, making systems smarter, more adaptive, and increasingly capable of learning from data over time.

Types of Artificial Intelligence Based on Capabilities

1. Narrow AI (Weak AI):

This is the most common type of artificial intelligence used today. It is designed to handle specific tasks and functions within a well-defined boundary. Examples include voice assistants like Siri or Alexa, facial recognition systems, and recommendation algorithms on streaming platforms. While effective at what it's designed to do, narrow AI doesn't possess general understanding or awareness beyond its specific application.

2. General AI (Strong AI):

General AI refers to a more advanced, yet still largely theoretical, form of AI. Unlike narrow AI, general AI would be able to understand, learn, and apply knowledge across a wide range of tasks just like a human. It would have the ability to reason, solve unfamiliar problems, and adapt to new situations without being pre-programmed for each one.

3. Superintelligent AI:

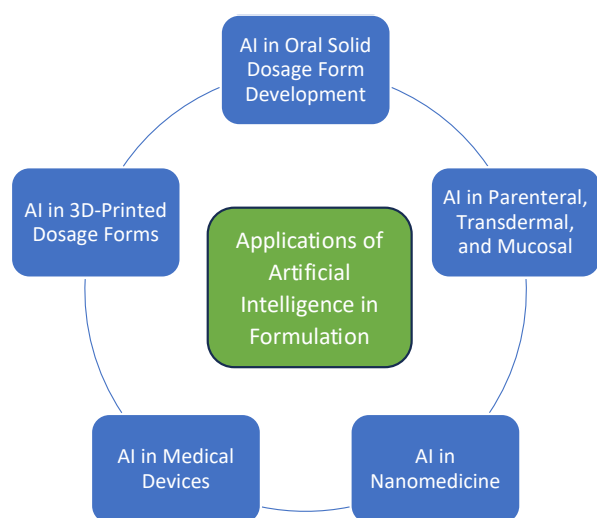
This form of AI remains speculative and has not yet been achieved. It describes a level of intelligence that far exceeds human capabilities in virtually every field scientific creativity, general wisdom, and even emotional intelligence. While it holds exciting possibilities, superintelligent AI also raises serious ethical, safety, and philosophical concerns, and is a major topic in AI ethics and governance discussions.



Table : 1) Conventional formulation V/S AI- Based formulation

Criteria	Conventional 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	Tends to be time-consuming, involving multiple rounds of manual testing.	Speeds up development by quickly simulating outcomes and reducing 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.
Personalization	Limited ability to customize formulations for individual patient needs.	Supports tailored treatments by analysing patient-specific data for personalized medicine.
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 Artificial Intelligence in AI in Oral Solid Dosage Form Development Formulation Development

**Figure 1: Application of AI in formulation development**

Artificial Intelligence (AI) is transforming how tablets and other solid dosage forms are developed in the pharmaceutical industry. It helps optimize formulations, reduce trial-and-error, save time, and lower costs. Techniques like Artificial Neural Networks (ANNs) and random forest algorithms are used to predict drug stability, dissolution patterns, and release profiles with high accuracy.

AI enables better understanding of how ingredients and process conditions affect tablet quality. It also supports decision-making by linking input parameters to desired product outcomes. However, as AI becomes more common in drug development, regulatory frameworks like

cGMP need to adapt to ensure product safety and consistency.

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 in Nanomedicine

Artificial Intelligence (AI) is significantly advancing the field of nanomedicine by improving the design, development, and application of nanoparticles for drug delivery, diagnostics, and personalized treatments. AI helps predict the behaviour, stability, and safety of nanoparticles, enabling researchers to create more effective and targeted therapies, especially for complex diseases like cancer.

Machine learning models can simulate drug release, optimize formulation parameters, and reduce the need for repeated lab experiments. AI is also used in real-time monitoring tools like nano-sensors to track drug levels or disease progression. These innovations support faster development and better patient outcomes.

AI in Parenteral, Transdermal, and Mucosal Drug Delivery

AI is helping improve complex drug delivery systems like injectables, patches, and mucosal products by optimizing formulation parameters (e.g., pH, solubility, stability) and manufacturing processes. It ensures better quality control, predicts product behaviour, and reduces trial-and-error.

AI is also used for particle inspection, detecting defects, and maintaining equipment. In transdermal and mucosal systems, AI and simulations allow smarter, faster, and more cost-effective formulation design, enabling personalized and efficient drug delivery.

AI in Medical Devices :

Artificial Intelligence (AI) is playing a major role in transforming medical devices, making healthcare smarter, more efficient, and personalized. With the rise of personalized care and remote health monitoring especially after the COVID-19 pandemic AI technologies have become even more essential.

Here's how AI is being used in different types of medical devices:

- **Helping with Diagnoses:** AI can examine medical images like X-rays, CT scans, or MRIs and assist doctors in identifying diseases such as cancer or heart problems with greater accuracy and speed.
- **Remote Health Monitoring:** Devices powered by AI can track patients' vital signs in real-time from their homes. This is especially helpful for people with chronic conditions. The data collected is analysed instantly, allowing healthcare providers to respond quickly if something seems off.
- **Wearable Health Gadgets:** Smartwatches, fitness bands, and biosensors now include AI to monitor health factors like heart rate, sleep



cycles, physical activity, and even blood sugar. These gadgets offer users helpful insights and tips to manage their health better.

- **Prosthetics and Physical Therapy:** Advanced prosthetic limbs use AI to mimic natural movement by learning from the user's motions. In rehabilitation, AI tracks and analyses a patient's progress and gives real-time feedback to improve movement and recovery.
- **Assisting in Surgery:** AI is also used in robotic surgical tools to help doctors perform surgeries with high precision. It can process data during surgery to offer suggestions or alerts, which improves patient safety and surgical results.
- **Managing Medications:** Smart pill dispensers powered by AI remind patients when to take their medicine, ensure correct dosages, and track whether medications are being taken regularly. AI can also personalize medication schedules based on health data and treatment history.^[1]

Limitations of AI in Drug Development

Artificial Intelligence (AI) has transformed many parts of pharmaceutical research and drug development. From predicting drug interactions to identifying promising molecules, its contributions are impressive. But like any powerful tool, AI has its limitations and understanding them is essential to using it wisely.

1. It's Still a "Black Box"

Many AI models are so complex that even their creators can't always explain how they come to certain decisions. This lack of transparency makes it difficult for regulators and scientists to fully trust the results, especially when predictions don't align with medical expectations. Trust is hard to build if

we can't clearly explain the "why" behind AI decisions.

2. Not Enough or Poor-Quality Data

AI learns best from large amounts of good-quality data. But for some conditions especially rare diseases there simply isn't enough data to train reliable models. In other cases, the data might not represent the full population, leading to results that work for some people but not for others.

3. Bias in Data Can Skew Results

If the training data is biased for example, if it overrepresents certain age groups, genders, or ethnicities then the AI will also be biased. That could mean the model fails to predict how a drug works for underrepresented groups, which can lead to unsafe or ineffective treatments.

4. Difficult to Keep Up with New Information

Once an AI model is built, updating it with new discoveries or clinical data isn't always easy. In a field like pharmaceuticals, where new information is constantly emerging, this makes it hard for AI to stay relevant without significant time and effort to retrain the model.

5. May Not Handle Individual Differences Well

AI models often work based on average responses in large datasets. But real patients don't always behave like averages. Especially in diseases like cancer, where every patient responds differently, AI might miss the mark in predicting how a treatment will work for a specific person.

6. Results Can Be Hard to Understand

Even when AI delivers useful predictions, the results can be difficult to interpret. Clinicians and researchers might struggle to translate those



outputs into real-life decisions, especially if they aren't trained in how AI works.

7. Privacy and Ethical Issues

AI systems often rely on sensitive personal health data, which raises serious questions about privacy and data ownership. It's crucial that patient information is handled responsibly, with clear guidelines on how data is collected, stored, and used.

8. Biology Is Too Complex for Simple Models

Our bodies are incredibly complex, and AI models no matter how advanced can't always capture every interaction or variable. Small changes in genetics, environment, or health status can make a big difference in how a drug works, and these subtleties aren't always reflected in AI predictions.

9. AI Can't Replace Human Judgment

While AI is great at spotting patterns, it doesn't understand the context or emotion behind medical decisions. Doctors consider many factors beyond data like a patient's history, lifestyle, and preferences when making treatment choices. AI doesn't yet have that depth.

10. Inaccurate Predictions for Drug Molecules

AI is often used to predict which molecules might bind to a target protein. But sometimes, the simulations get it wrong, either missing effective compounds or falsely identifying inactive ones. This makes experimental testing still essential, even when AI offers predictions.^[1]

Machine Learning

Machine Learning (ML), a branch of Artificial Intelligence (AI), involves the use of computer algorithms that can analyse and learn from data on their own without needing explicit programming for each specific task. These algorithms are capable of solving problems, making predictions, and supporting better decision-making by continuously improving through experience.

Machine Learning Workflow in Drug Formulation

Machine Learning Workflow in Drug Formulation (Summary)

The machine learning (ML) process in drug formulation follows a structured workflow to ensure accurate and reliable outcomes. It starts with collecting relevant data such as particle size, solubility, and tablet hardness and organizing it for analysis. When complete datasets aren't available from single studies, researchers often combine information from published sources. Before training, the data is cleaned and sometimes clustered to detect early trends. It is then divided into three parts: training (to teach the model), validation (to fine-tune it), and testing (to assess its performance on new data).

The model's effectiveness is evaluated using tools like RMSE for prediction accuracy or KNN for classification. If data is limited, techniques like cross-validation help improve reliability. After training, the model is analysed to identify which features influenced outcomes the most, guiding future formulation strategies.



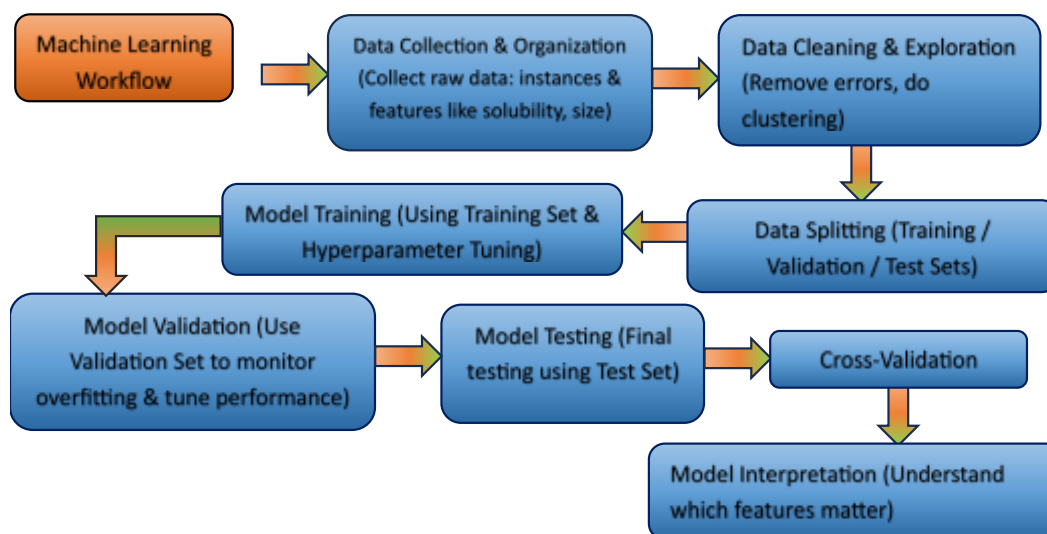


Figure 2 : Machine learning workflow

There are two categories of ML :-

1. Supervised Learning :

Supervised learning is a method where the machine is trained using data that already has correct answers, or "labels." The system learns by example it looks at the input data along with the known results and tries to figure out how they're connected. Once trained, it can use this knowledge to predict outcomes when it sees new data.

Example: Think of a program trained to recognize animals in pictures. If you give it thousands of images labelled as "dog," "cat," or "bird," it learns the differences and can then correctly identify animals in brand-new, unlabelled photos.

2. Unsupervised Learning :

In unsupervised learning, the machine is given data without any labels there are no correct answers provided. The model's job is to explore the data on its own and find patterns or groupings that might not be obvious. It's like giving the system a puzzle and asking it to figure out how things fit together without any instructions.

Example: A retailer might use unsupervised learning to group customers based on their shopping habits, even if there's no predefined category. This helps in creating personalized marketing strategies.

Table : 2) Supervised V/S Unsupervised ML ^[2]

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)
Interpretability	Easier to interpret and validate due to known outcomes	Can be harder to explain findings might need additional context
Performance Focus	High accuracy in predicting specific outcomes	Good for discovering trends or organizing large data sets
Common in Drug Formulation?	Yes widely used to predict or optimize formulation outcomes	Occasionally used for exploratory purposes or when relationships between data points are unclear
Example Case Studies	Predicting nanoparticle size using deep learning; classifying tablet quality with decision trees	Clustering disintegration behaviours using Kohonen SOM networks

Applications of Machine Learning in Pharmaceutical Formulation

Enhancing Formulation Through Machine Learning :

Developing a medicine involves selecting the right mix of active ingredients and excipients (the substances that help deliver the drug effectively). Traditionally, this process depended on a lot of guesswork, involving repeated testing and adjustments which can be slow and expensive. Machine Learning (ML) has changed this by offering a faster, smarter way to improve formulations.

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.

Speeding Up the Discovery of Optimal Formulations :

Creating the perfect drug formulation requires considering many variables such as how

ingredients interact, how the drug is absorbed in the body, and how it's manufactured. Previously, scientists had to rely on a slow process of trial and error. ML now helps speed this up significantly. ML can analyse huge amounts of past formulation data to predict how a new combination might perform. This predictive power helps scientists avoid unnecessary experiments, reducing the time and cost involved in developing new drugs.

Moreover, traditional formulation methods usually explore changes one step at a time. In contrast, ML can evaluate a broad range of options simultaneously, revealing combinations that may not have been tested otherwise. This means faster innovation and more effective formulations which ultimately benefit both manufacturers and patients.^[3]

Limitations of ML :

The use of machine learning in the pharmaceutical industry is often slowed down by problems with data quality and consistency. Since information comes from many different sources and formats, it is difficult to maintain uniform standards. The absence of clear data collection guidelines and the variation in quality practices across organizations make it harder to build reliable ML models. On top of that, combining old legacy records with today's digital platforms is still a big challenge, which



holds back the wider use of machine learning in drug research and development.⁽⁴⁾

Meeting regulatory requirements while adopting advanced machine learning solutions remains a complex task. Existing regulations are often not fully equipped to address the unique challenges posed by ML-driven pharmaceutical development, leading to uncertainty in model validation and approval. Since these systems are dynamic and continuously learning, ensuring long-term regulatory compliance becomes even more difficult. On the technical side, implementing ML requires powerful computing resources and advanced infrastructure, which many organizations find costly to maintain and upgrade. Along with this, integrating ML tools with existing systems while safeguarding sensitive data continues to be a persistent challenge.⁽⁵⁾

The adoption of machine learning in pharmaceutical development brings forward several ethical concerns, particularly around data privacy, algorithmic bias, and transparency in decision-making. It is essential to ensure that training datasets are representative and unbiased to avoid skewed outcomes. At the same time, keeping human oversight in critical decision-making processes is vital to maintain accountability and trust.⁽⁶⁾

Impact of AI and ML on the Drug Development Pipeline

Artificial Intelligence (AI) and Machine Learning (ML) are significantly reshaping how new drugs are developed. These advanced technologies are now being applied across every stage of the drug development process, offering faster and more accurate screening of potential compounds, precise prediction of drug properties, and intelligent optimization of formulation components. This not only accelerates the

discovery process but also reduces the need for repetitive testing saving both time and resources.

Beyond enhancing speed and efficiency, AI and ML are enabling a shift toward personalized medicine. By analysing patient-specific data, these tools help tailor drug dosages and predict individual treatment responses, making therapies more effective and safer. In the early stages of drug development, AI can also identify possible side effects or adverse reactions, allowing for proactive risk mitigation.

Furthermore, the integration of AI/ML into pharmaceutical operations brings about cost reduction and greater productivity. Automated systems and data-driven decision-making streamline complex processes, improve consistency, and reduce human error. This leads to higher overall efficiency, helping pharmaceutical companies remain competitive in a rapidly evolving landscape. These capabilities are transforming drug development from a traditionally slow and costly process into a smarter, more agile system that can deliver better outcomes for both developers and patients.^[7]

Additionally, researchers highlight that AI's growing role extends from early-stage discovery all the way to clinical application truly bridging the gap from the laboratory bench to bedside care.^[8]

Key Components in Artificial Intelligence and Machine Learning

Neural Networks :

Neural networks are designed to work like the human brain they're systems of algorithms that can detect patterns and connections within large and complex datasets. One advanced form, called deep learning, uses many layers of these networks to analyse detailed information, such as images,



speech, and text. These models are especially powerful when dealing with high-dimensional data, helping AI systems make accurate and intelligent predictions.

Natural Language Processing (NLP) :

Natural Language Processing, or NLP, is what allows computers to understand and respond to human language both written and spoken. It plays a big role in making interactions with technology feel more natural.

Example: When you ask Siri or Alexa a question, it's NLP that helps them understand your words and respond appropriately.

Computer Vision :

Computer vision gives machines the ability to "see" and make sense of visual content like images or video. By analysing this input, AI systems can recognize faces, detect objects, or even understand scenes.

Example: Facial recognition apps and image-based security systems rely heavily on computer vision technology.

Data Mining :

Data mining involves sifting through huge amounts of information to find useful patterns, relationships, or trends. Machine learning algorithms make this process more powerful by learning from the data and providing predictive insights. It's widely used in industries to make informed decisions based on data-driven evidence.^[9]

Formulation Stability Assessment Using AI and Machine Learning

Accelerated Stability Studies :

Accelerated stability testing plays a vital role in pharmaceutical formulation. It involves storing drug products under extreme conditions such as elevated temperatures and humidity to predict how they will behave over long-term storage. Traditionally, this method was used to estimate degradation and shelf life. However, with the help of Artificial Intelligence (AI) and Machine Learning (ML), this process has become much smarter and more efficient.

AI and ML tools can analyse large amounts of experimental data, spot hidden patterns, and predict how and when a drug might degrade. These technologies also help identify what factors affect stability the most. As a result, scientists can make better decisions, optimize formulations early, and more accurately determine expiration dates saving time and reducing the need for repeated testing.

2. Prediction of Degradation Pathways :

Knowing how a drug breaks down over time is crucial to ensure it stays safe and effective. Machine Learning algorithms like neural networks and decision trees are now being used to predict possible degradation processes, such as chemical breakdown due to moisture (hydrolysis) or exposure to oxygen (oxidation).

These models work by studying relationships between a drug's chemical structure, the excipients it's combined with, and environmental factors from testing. They provide scientists with valuable insights to make necessary changes to a formulation to improve its stability. When paired with expert knowledge about drug chemistry, these predictions become even more accurate and easier to understand.

3. Shelf-Life Prediction :



AI and ML have also transformed how shelf life is predicted. These tools can process extensive data about a drug's ingredients, storage conditions, and how it breaks down over time. By doing so, they help forecast how long a product will remain effective and safe.

This predictive ability is not only useful for product development but also crucial for meeting regulatory standards. In addition, using AI during early development stages can prevent stability issues from arising later. Combined with statistical methods and expert insights, these models ensure a drug's shelf life is both reliable and scientifically validated.^[10]

Success Stories and Challenges in AI-Based Drug Formulation

The pharmaceutical industry is increasingly turning to Artificial Intelligence (AI) and Machine Learning (ML) to improve how drugs are developed and formulated. Companies like Pfizer and Atomwise are leading the way. Pfizer's *Centaur Chemist* platform is being used to forecast chemical reactions and refine synthetic pathways, while Atomwise's *AtomNet* technology is identifying potential new treatments for serious illnesses, including Ebola, multiple sclerosis, and even COVID-19. AI is also proving valuable in rare disease research, helping uncover possible therapies for conditions like Angelman syndrome.

However, despite these encouraging developments, several challenges remain. A major hurdle is the limited availability of high-quality, comprehensive data especially during the early phases of research. This can affect the performance and reliability of AI models. In addition, many advanced AI systems, particularly those using deep learning, are often viewed as "black boxes" because their decision-making processes are difficult to understand or explain.

There are also significant regulatory and ethical concerns. Questions about data privacy, patient consent, and algorithmic fairness are increasingly important and must be addressed through strict regulatory oversight.^[11]

To overcome these issues, it's crucial to improve how data is collected, organized, and shared across the industry. Close collaboration among scientists, regulatory bodies, and industry professionals will be essential for developing transparent guidelines that ensure AI tools are both reliable and ethical. With the right frameworks in place, AI and ML can become powerful, trustworthy allies in advancing pharmaceutical research and drug development.^[12]

Future Prospects and Emerging Trends in AI/ML for Pharmaceuticals

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.

Another exciting development involves the use of transfer learning and domain adaptation, which allow pre-trained AI models to be fine-tuned for specific pharmaceutical applications. This not only cuts down on training time but also improves the model's performance and flexibility in real-world drug development scenarios. Equally important is the emergence of explainable AI (XAI) a growing priority in the pharmaceutical field. As AI systems become more integrated into regulated



environments, such as healthcare and drug development, there's an increasing need for transparency. XAI ensures that the logic behind AI decisions is understandable and justifiable to both scientists and regulatory authorities. Generative models, like Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs), are also gaining traction. These innovative tools can design entirely new molecular structures, opening doors to the discovery of novel drug candidates with optimized properties dramatically speeding up the early phases of drug development.^[13]

Looking ahead, the field of pharmaceutical formulation and technology is set for revolutionary change. With AI and ML becoming more integrated into every stage of research and development, we can expect smarter, faster, and more efficient approaches to drug creation. These advances promise to bring a new level of precision and innovation, shaping the future of personalized and effective medicine ^[14]

CONCLUSION

Artificial Intelligence (AI) and Machine Learning (ML) are rapidly transforming the landscape of pharmaceutical formulation and drug delivery. From simplifying early-stage drug discovery to optimizing complex formulations and enhancing personalized medicine, these technologies are reshaping how medicines are designed, developed, and delivered. By integrating data-driven insights, AI and ML reduce the reliance on traditional trial-and-error methods, making formulation development faster, more cost-effective, and more accurate. Applications range from oral solid dosage forms and nanomedicine to 3D printing, parenteral systems, and even intelligent medical devices. Machine learning workflows and neural networks now help researchers predict formulation outcomes, assess drug stability, and identify novel

therapeutic compounds. However, despite their vast potential, challenges remain such as data limitations, model transparency, algorithmic bias, and regulatory uncertainties. Ethical concerns around privacy and decision-making also require careful governance. Importantly, AI cannot replace human expertise but serves as a powerful tool to enhance scientific understanding and decision-making.

Looking ahead, the future of AI in pharmaceuticals is incredibly promising. With advancements in explainable AI, deep learning models, and real-time data integration, pharmaceutical sciences are entering an era of smarter, more personalized healthcare. The continued collaboration between scientists, regulators, and technologists will be crucial in unlocking the full potential of AI and ML ultimately improving treatment outcomes and shaping the next generation of drug development.

REFERENCES

1. Vora, L. K., Gholap, A. D., Jetha, K., Thakur, R. R. S., Solanki, H. K., & Chavda, V. P. (2023). Artificial Intelligence in Pharmaceutical Technology and Drug Delivery Design. *Pharmaceutics*, 15(7), 1916.
2. Gupta, A., Vaidya, K., & Boehnke, N. (n.d.). AI and machine learning in pharmaceutical formulation and manufacturing of personalized medicines. Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, United States.
3. Dangeti, A., Bynagari, D. G., & Vydani, K. (n.d.). Revolutionizing drug formulation: Harnessing artificial intelligence and machine learning for enhanced stability, formulation optimization, and accelerated development. Pydah College of Pharmacy, Patavala; Koringa College of Pharmacy, Korangi.



4. Danysz K, Cicirello S, Mingle E, et al. Artificial intelligence and the future of the drug safety professional. *Drug Saf.* 2019;42(4):491-497.
5. Fleming N. How artificial intelligence is changing drug discovery. *Nature.* 2018;557(7706):S55-S57.
6. Blasimme A, Vayena E. The ethics of AI in biomedical research, patient care, and public health. *Oxford Handbook of Ethics of Artificial Intelligence.* 2020:703-718
7. Paul, D., Sanap, G., Shenoy, S., Kalyane, D., Kalia, K., & Tekade, R. K. (2021). Artificial intelligence in drug discovery and development. *Drug Discovery Today*, 26(1), 80–93.
8. Vidhya, K. S., Sultana, A., Kumar, N., Rangareddy, H., Vidhya, K. S., & Madalageri, N. K. (2023, October 22). Artificial Intelligence's Impact on Drug Discovery and Development: From Bench to Bedside. *Cureus*, 15(10).
9. Jena, G. K., Patra, C. N., Jammula, S., Rana, R., & Chand, S. (2024). Artificial Intelligence and Machine Learning Implemented Drug Delivery Systems: A Paradigm Shift in the Pharmaceutical Industry. Department of Pharmaceutics, Roland Institute of Pharmaceutical Sciences, Berhampur, Odisha, India. Retrieved from
10. 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. Lloyd Institute of Management and Technology, Greater Noida, Uttar Pradesh, India 201306. *International Journal of Newgen Research in Pharmacy & Healthcare*, 2(1).
11. World Health Organization. (2021). Ethics and governance of artificial intelligence for health: WHO guidance.
12. Dangeti, A., Bynagari, D. G., & Vydani, K. (n.d.). Revolutionizing drug formulation: Harnessing artificial intelligence and machine learning for enhanced stability, formulation optimization, and accelerated development. Pydah College of Pharmacy, Patavala; Koringa College of Pharmacy, Korangi.
13. Askr, H., Elgeldawi, E., Aboul Ella, H., Elshaier, Y. A., Gomaa, M. M., & Hassanien, A. E. (2023). Deep learning in drug discovery: An integrative review and future challenges.
14. Dangeti, A., Bynagari, D. G., & Vydani, K. (n.d.). Revolutionizing drug formulation: Harnessing artificial intelligence and machine learning for enhanced stability, formulation optimization, and accelerated development. Pydah College of Pharmacy, Patavala; Koringa College of Pharmacy, Korangi.

HOW TO CITE: Anuja Ghaywat, Ramdas Darade, Vikram Saruk, Manoj Garad, Swati Gaykar, Priti Bhure, Komal Gunjal, AI and Machine Learning in Formulation Development, *Int. J. of Pharm. Sci.*, 2025, Vol 3, Issue 10, 1199-1211. <https://doi.org/10.5281/zenodo.17339741>

