

**A REVIEW ON: THE IMPACT OF ARTIFICIAL INTELLIGENCE IN FORMULATION DEVELOPMENT****Sandip Kumar Tiwari, Vipul Singh and Sanjay Kumar Kushwaha\***

Bhavdiya Institute of Pharmaceutical Sciences and Research, Ayodhya, Uttar Pradesh.

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**\*Corresponding Author**  
**Sanjay Kumar Kushwaha**Bhavdiya Institute of  
Pharmaceutical Sciences  
and Research, Ayodhya,  
Uttar Pradesh.**ABSTRACT**

AI has become a game-changing instrument that uses human knowledge to solve difficult problems with previously unheard-of levels of efficiency. Artificial intelligence (AI) and machine learning technologies have completely changed the pharmaceutical sciences, including drug development, formulation, and dosage form testing. Scientists are able to determine disease targets and anticipate interactions with possible treatment candidates by using artificial intelligence (AI) algorithms to analyse large biological datasets like proteomics and genomes. By improving the accuracy and speed of drug discovery, this strategy raises the possibility that a medicine will be approved. Additionally, AI lowers research and development costs by streamlining procedures, helping with trial planning, forecasting pharmacokinetics, and assessing toxicity at an early stage of development. This feature reduces the need for time-consuming and

expensive animal testing by streamlining the lead compound optimisation and prioritisation process. By analysing real-world patient data, AI also helps personalised medicine by enabling the development of individualised treatment plans that increase patient adherence and efficacy. This thorough analysis examines the many uses of AI in pharmaceutical technology, including pharmacokinetics/pharmacodynamics (PK/PD) research, dosage form design, process optimisation, and drug discovery. The paper addresses several AI-based strategies, highlighting their advantages while also pointing out any potential drawbacks. The pharmaceutical business has great opportunities to improve patient care and advance drug development processes via further investment and investigation of AI.

**KEYWORDS:** Artificial intelligence (AI), Drug discovery, Drug delivery, Machine learning, Era of machines, Algorithm, Machine learning, Nano medicine, Nano robots,

Pharmaceutical formulation, Drug development.

## 1. INTRODUCTION

Using a variety of approaches, several industries are working to accelerate their development in order to satisfy the needs and expectations of their clients. The pharmaceutical sector is an important one that is essential to preserving lives. It functions by means of constant innovation and the assimilation of novel technologies in order to tackle worldwide healthcare issues and react to medical crises, like the last epidemic.<sup>[1]</sup>

Innovation in pharmaceuticals is usually based on a great deal of research and development in a number of areas, such as packaging, customer-focused marketing techniques, and manufacturing technologies.<sup>[2]</sup>

Small molecule drugs and biologics are examples of novel pharmaceutical developments. Better stability and high potency are preferred to address unmet needs in disease treatment. A great deal of anxiety surrounds the evaluation of the substantial levels of toxicity linked to novel medications, which will require in-depth investigation and study in the near future. Providing medication molecules with the best possible benefits and suitability for use in the healthcare sector is one of the main goals. In spite of this, the pharmacy sector encounters many challenges that need for additional development utilizing technology-driven approaches to meet global medical and healthcare demands.<sup>[3-5]</sup>

The healthcare sector is always in need of skilled workers, thus educating healthcare staff on a regular basis is necessary to enhance their participation in daily tasks. Within the pharmaceutical sector, identifying skill shortages in the workplace is a critical undertaking. Although it might be difficult to provide enough training, it is crucial to address the deficiencies that have been found and take the necessary corrective action. According to a report that was given by some Furthermore, it has been noted that June 2022 had almost 41% of supply chain interruptions. The research goes on to say that supply chain disruption has been identified as the second most difficult obstacle to overcome. In order to improve company resilience, a number of pharmaceutical businesses are looking forward to new developments in their supply chains and creative approaches to these problems.<sup>[6]</sup> Numerous global operations, including current clinical studies, have been severely disrupted by the coronavirus disease epidemic of 2019 (COVID-19).<sup>[7]</sup>

Supply chain disruptions are made worse by pandemics, natural disasters, price adjustments, cyberattacks, delays in logistics, and problems with products. The epidemic's effects on transport have wreaked havoc on global companies and the supply chain. Price fluctuation delays are caused by decision-induced delays for price updates from suppliers due to misunderstandings about whether to use the new price or the current price for commodities or materials. Countries' tactics for collaborating on cross-border commerce give birth to new challenges, including a growth in criminal activity and unstable supply of essential resources for production and operation. Customized footprints must be manufactured to meet patient requirements and ensure compliance.

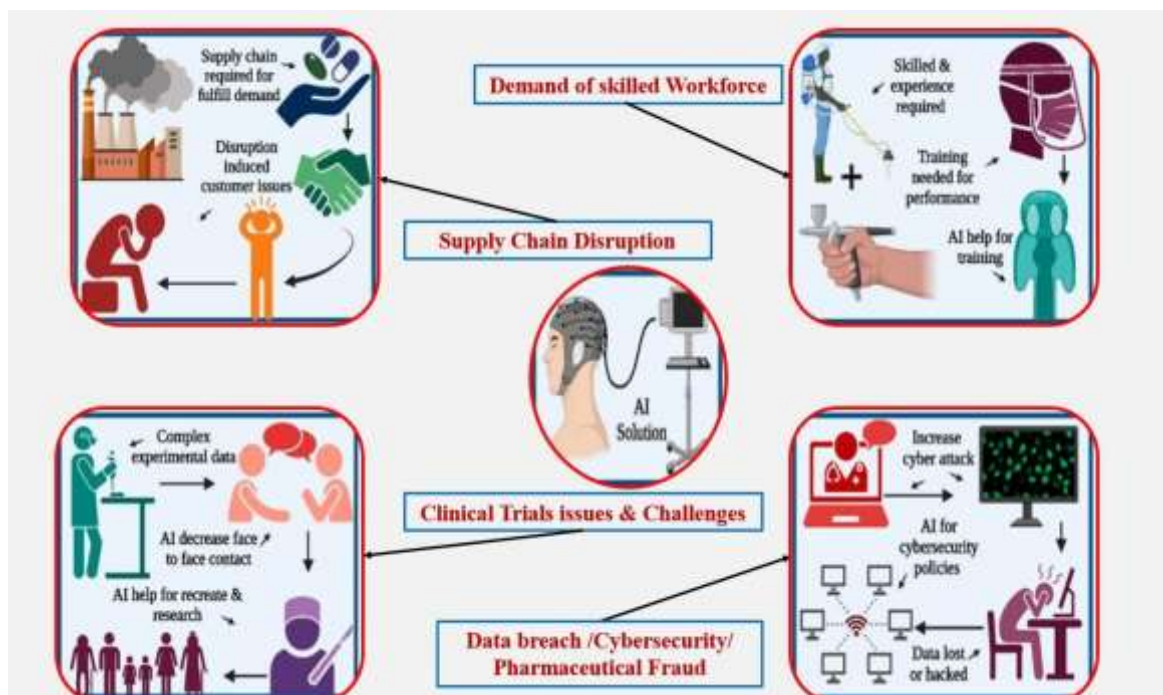
A large number of COVID-19 vaccinations produced by the pharmaceutical industry were rendered useless during the pandemic because to issues with cold chain maintenance. The main reason for the disruption of the supply chain that came about as a result of the delayed response is that industrial and commercial operations lack innovation and make inaccurate forecasts. Disruptions to the pharmaceutical industry's supply chain can have a big impact on prospective revenues, business reputation, and customer happiness.<sup>[8,9]</sup>

Supply chain activities in the pharmaceutical business are going to undergo a major change due to the introduction of artificial intelligence (Figure 1). Additionally, it synthesizes a multitude of AI research projects from the past few decades in order to produce practical answers for various supply chain problems. The paper also makes recommendations for future research directions that can improve supply chain management decision-making tools.<sup>[10,11]</sup>

The pandemic's main effects are starting to fade, although clinical studies are still impacted in some ways. A large number of pharmaceutical businesses are interested in using more modern technology, including artificial intelligence (AI) and virtual platforms. With less engagement for face-to-face kinds, these new technologies might be useful in restarting or recreating these clinical studies<sup>[12–18]</sup>, as shown in **Figure 1**.

Applying AI to research design facilitates both optimisation and accumulation for the tasks associated with developing a patient-centric design. Artificial Intelligence (AI) employs methods to gather the vast quantities of data produced by those clinical studies, which minimizes the need for human data collecting. By combining wearable technology with body sensors, these technologies enable remote recording of a patient's vital signs and other important data. This helps satisfy the patient's need for regular in-person connection. Real-time

insights are provided during the study process by wearable AI algorithms.<sup>[19]</sup>



**Figure 1: - illustrates a potential artificial intelligence (AI) remedy for the problems facing the pharmaceutical industry: all industries need to have skilled workers in order to take use of their knowledge, skills, and ability to innovate new products. The second deals with issues related to disruptions in the supply chain and clinical trial experiments. Cyberattacks are becoming more common, and security and data breaches are becoming major issues for business.**

#### [A] Overview of traditional Methods in formulation development

In the pharmaceutical business, traditional formulation development is a methodical procedure that turns an API (Active Pharmaceutical Ingredient) into a finished drug that can be given to patients in a safe and efficient manner.<sup>[20]</sup>

#### • Here Several Key Stages

##### I. Pre-formulation Studies

The physical and chemical characteristics of the API are being characterized at this first stage. The evaluation of crucial factors including stability, compatibility with excipients, and solubility helps determine how an API will act in a formulation.<sup>[21]</sup>

## II. Formulation Design

Different formulation techniques are devised and assessed based on pre-formulation data. This involves choosing the right excipients, or inactive substances, to help the API be delivered, stable, and palatable. Prototypes are created and various dosage forms—such as pills, capsules, injections, etc.—are taken into consideration.<sup>[21]</sup>

## III. Optimization and Screening

Formulation prototypes undergo screening and optimization in order to attain the targeted attributes, including stability, manufacturability, and bioavailability. Iterative testing and improvement are frequently used in this phase to strike a balance between patient compliance, safety, and efficacy.<sup>[21]</sup>

## IV. Scale-Up and Manufacturing

The method is scaled up from laboratory to pilot and finally to full-scale manufacturing if an ideal formulation has been found.<sup>[22]</sup> Making sure the formulation can be manufactured reliably and economically at bigger scales is part of this.<sup>[22]</sup>

## V. Quality Control and Stability Testing

Strict quality control procedures are carried out to guarantee that the finished product satisfies all legal requirements. To find out how long a product will last on the shelf and to make sure it stays safe and effective for the duration of its intended use, stability testing is done.<sup>[23]</sup>

## VI. Regulatory Approval

The finished product is well documented before being submitted for approval to regulatory bodies. This entails proving the product's efficacy, safety, and quality through clinical trials and other necessary research.<sup>[23]</sup>

## [B] Introduction to AI and its relevance to pharmaceuticals

The simulation of human intelligence in computers created to think and learn like humans is known as artificial intelligence, or AI. AI is transforming medication development, discovery, and personalized therapy in the pharmaceutical industry. Predictive modelling, automated synthesis, virtual screening, and clinical trial design optimization are some of its uses. AI improves patient outcomes by streamlining pharmaceutical research, cutting expenses and time, and increasing the precision of treatment procedures.<sup>[24,25,26]</sup>

## 2. Current Pharmaceutical Challenges and AI Technologies in Pharmaceutics formulation

### I. Machine Learning (ML) in Pharmaceutics

Algorithms and statistical models are used by machine learning (ML), a branch of artificial intelligence (AI), to analyse and comprehend intricate data patterns. And shown in **figure 2**.

*In pharmaceutics, ML is instrumental in several key areas*

#### a). Drug Discovery

Early on in the drug development and design process is one of the most important areas where machine learning is being used in pharmaceutics. ML algorithms are more effective than conventional techniques at identifying possible drug candidates by analysing vast databases of chemical substances and biological targets.<sup>[27]</sup>

- **Virtual Screening:** By predicting a compound's biological activity, machine learning models allow for the virtual screening of large chemical libraries in order to find potential therapeutic candidates.<sup>[27]</sup>
- **De Novo Drug create:** By using machine learning to generate novel chemical structures that are likely to be effective, ML can help create new molecules with desired attributes.<sup>[27]</sup>
- **Predictive Modelling:** Drug safety and efficacy depend on the ability of algorithms to forecast pharmacokinetic and pharmacodynamic features such toxicity, absorption, distribution, metabolism, and excretion (ADME).<sup>[27]</sup>

#### b). Preformulation Studies

Preformulation studies are conducted to characterise the physicochemical properties of drugs in order to provide information for formulation decisions. Through formulation optimisation and important property prediction, ML can improve this research.<sup>[28]</sup>

- ✚ **Solubility Prediction:** A key component of designing efficient drug delivery systems is the ability of machine learning models to forecast a drug candidate's solubility in a range of solvents.
- ✚ **Stability Analysis:** By predicting a pharmacological compound's stability in various scenarios, algorithms can assist find probable degradation pathways and enhance formulation stability.
- ✚ **Bioavailability Prediction:** ML can predict a drug's bioavailability based on its molecular



characteristics, which helps choose the best delivery system.<sup>[28]</sup>

### c). Formulation Optimization

Optimisation algorithms and ML-driven design of experiments (DoE) can greatly enhance the formulation development process by the software and AI Tools present in **Table no 1**.

- ❖ **Excipient Selection:** ML eliminates the need for lengthy trial-and-error testing by determining the best mix of excipients to improve drug stability, solubility, and bioavailability.<sup>[28]</sup>
- ❖ **Process Optimisation:** By forecasting how different process factors will affect product quality and yield, algorithms can optimise production processes, resulting in more effective and repeatable formulas.<sup>[28]</sup>

### d). Quality Control and Assurance

In order to guarantee the consistency and quality of pharmaceutical products, machine learning is essential.

🔧 **Predictive Maintenance:** By using ML models to forecast maintenance requirements and equipment breakdowns, downtime can be reduced and uninterrupted production can be guaranteed.

🔧 **Real-Time Monitoring:** Algorithms are able to detect and ensure the quality of the product by analysing data in real-time from sensors and other monitoring devices.<sup>[28]</sup>

## II. Deep Learning (DL) in AI Technologies in Pharmaceutics

Multiple-layered neural networks are used in Deep Learning (DL), a specialised subfield of Machine Learning (ML), to analyse complex data structures.<sup>[29]</sup>

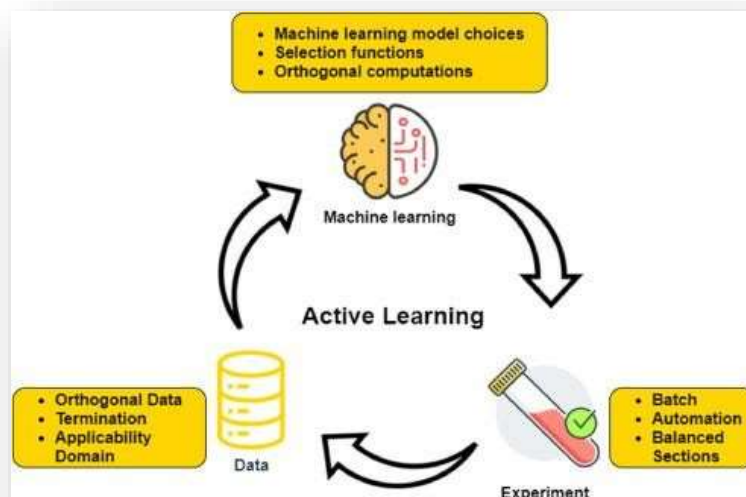
### DL has transformational applications

a). **Drug development:** By identifying novel drug candidates, forecasting their interactions, and optimizing molecular attributes, DL models may analyse large chemical and biological datasets, greatly improving the drug discovery process.<sup>[30]</sup>

b). **Biomarker Identification:** To help in the development of tailored therapeutics, DL algorithms examine genomic, proteomic, and metabolomic data to find biomarkers for illness diagnosis, prognosis, and therapeutic response.

c). **Image Analysis:** DL is an expert in medical image analysis, helping with advanced imaging methods like MRIs, CT scans, and histopathology to help diagnose and track diseases.

**d). Natural Language Processing (NLP):** DL-enabled NLP tools enable thorough data mining and knowledge discovery by extracting insightful information from patents, clinical trial reports, and scientific literature.<sup>[31]</sup>



**Figure 2: - AI learning models/tools for pharmaceutical applications.**

**Table 1: - Top 4 list of commonly used AI models in the pharmaceutical industry.**

AI Based Machine Learning Models	Description and Usage	References.
<b>GANs</b> (Generative Adversarial Networks)	In order to produce unique chemical compounds and optimise their attributes, GANs are commonly utilised in the creation of medicinal products. To generate structurally varied and functionally optimised drug candidates, GANs are composed of a discriminator network that assesses the quality of newly created molecules and a generator network that generates new ones.	[32]
<b>RNNs</b> (Recurrent Neural Networks).	In the process of developing new drugs, RNNs are frequently used for sequence-based tasks including peptide sequence design, protein structure prediction, and genomic data analysis. They are able to produce new sequences based on patterns they have learnt and grasp sequential interdependence.	[33]
<b>CNNs</b> (Convolutional Neural Networks)	CNNs work well for image-based applications like finding possible drug targets and analysing chemical structures. They can help with target discovery and drug design by extracting pertinent information from molecular pictures.	[34]
Autoencoders	In drug development, autoencoders are unsupervised learning models that are utilised for feature extraction and dimensionality reduction. They can help in compound screening and virtual screening as well as capture important features of molecules.	[35, 36]

### 3. AI Tool Application in Different Dosage Form Designs

To comprehend the effects of medication distribution, the human body system is separated into many compartments. Based on biological membranes, the compartments are further simplified.



Physicochemical barriers can be applied in accordance with the method of medication administration within the body and are essential for biological compartments. Based on the route of administration, the rate of penetration is one of the most important parameters for effective drug delivery system monitoring. Once the medicine is taken orally and reaches the stomach, it needs to pass through the intestinal or gastric epithelium. The drug's continued distribution into the circulation depends on this phase. The medicine is delivered to the target site—tissue or any of the several cellular components—during the distribution process.<sup>[37–38]</sup> Drugs can also target intracellular molecules to enter the body. Biological barriers, whether active or passive, assist the majority of medication penetration. The drug's molecular characteristics determine passive diffusion. Through computation analysis, the *in silico* models are utilised to forecast drug distribution; nevertheless, the outcomes deviate somewhat from the real drug distribution study.

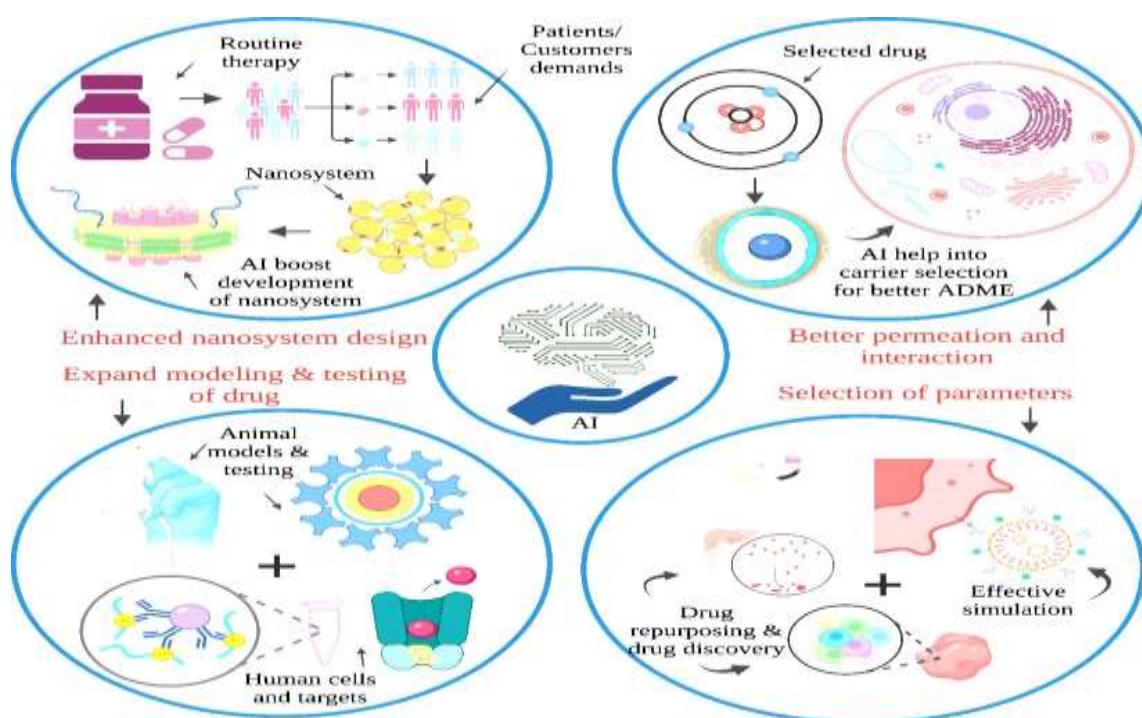
The way a medication behaves in the body is greatly influenced by its interactions with biological elements and its accessibility in biological settings. The molecular characteristics of the medication control this process. Passive permeation is ineffective for many tiny molecules and physiologically active substances, necessitating the use of a particular drug delivery mechanism. Membrane transport drives and intricate biological interactions are necessary for the active permeation process.

Studying the drug delivery system's pharmacokinetic characteristics is done with this more recent computer model. Preclinical models' predictability represents one of the biggest gaps in the pharmaceutical industry's research and development. Just like with complicated *in silico* models, the predictability assumption is predicated on the parameters that are chosen. **Figure 3** illustrates how the modelled environment may be used to analyse all of these scenarios, which are related to medication interactions with membranes. AI can help with the study and analysis of this simulated environment more successfully.<sup>[39–40]</sup>

The best results are determined by applying a methodical model and evaluating its parameters, taking into account various elements including simulation, scoring, and refining at every stage of the study process. AI may offer a solution that is automated and deployable for all of these purposes, enabling more accurate estimation and anticipated data refinement for continuous development.

As evidenced by the system biology type of the databases, a thorough grasp of the drug-biological interaction is necessary for improved AI training in the biological setting. Numerous cutting-edge AI tools, such as artificial neural networks, may be used to conduct pharmacokinetic investigations. In addition, AI offers a plethora of resources, including phenotypic, chemical, and genomic databases, to facilitate the efficient investigation of the intricate unit functions of molecules inside drugs and to improve comprehension of drug interactions. Some of the techniques are also used to investigate how the drug delivery system affects the medication's pharmacokinetics, which helps to effectively understand the toxicity and disposition of the drug.

Prior to conducting real trials, many novel methods to drug delivery systems entail designing quality and key qualities and assessing how they will affect the trials.



**Figure: - 3 AI's contribution to medication discovery and development. AI has applications in nano system design, drug discovery, and drug repurposing. It may also be used to expand the current drug testing modelling system. Understanding drug permeation, simulation, and human cell targets can also aid in improving comprehension of the mechanics of membrane interaction with the simulated human environment.**

AI uses what is known today to aid with applications in the future. It illustrates how artificial intelligence (AI) systems may manage and process enormous amounts of data to improve the

logical design of the product.

Improved self-supervised experimental outcomes and appropriate parameter recording are linked to a more rigorous codification within the knowledge base.<sup>[41-42]</sup>

#### **4. AI Used for Drug Delivery**

Computational pharmaceuticals, which improves medication delivery through multiscale modelling, is the result of pharmaceuticals' integration of AI and big data. By analysing massive information, AI and machine learning algorithms can anticipate drug behavior and optimise delivery methods.

This method minimises trial-and-error studies, which speeds up medication development, lowers costs, and boosts production.

Through the analysis of intricate correlations between drug characteristics, formulation elements, and physiological parameters, computational pharmaceuticals predicts drug transport from molecular interactions to macroscopic behavior. Designing effective drug delivery systems and forecasting physicochemical characteristics, in vitro release patterns, and drug stability are made easier with this thorough understanding. By detecting hazards and optimising medication performance early in development, artificial intelligence (AI) techniques enhance the assessment of in vivo pharmacokinetic parameters and in vivo-in vitro correlation studies. This reduces unanticipated results and resource-intensive tests.<sup>[43-44]</sup>

##### **4.1 AI used in Oral Solid Dosage Form Development**

To develop human-like skills, artificial intelligence (AI) uses sophisticated hardware and software. In several industries, including the pharmaceutical one, such innovation has been beneficial, particularly in the last few years during the product development stage. The time, money, and resources needed for production and efficient delivery to final consumers via the supply chain can be reduced by using these technical advancements. Furthermore, it offers an enhanced framework for comprehending how process characteristics affect product development and manufacture.

Redefining regulations addressing current good manufacturing practice (cGMP) is made more difficult for regulatory agencies by the use of AI. For the creation of stable dosage forms and a better comprehension of the inputs and outputs for processing and operations, several artificial intelligence (AI) technologies are used, including artificial neural networks (ANNs),

fuzzy logics, neural networks, and genetic algorithms. Solid dosage forms benefit from the usage of ANNs for improved prediction capabilities, whereas input parameter utilization results in the application of genetic algorithms for prediction.<sup>[45]</sup>

#### 4.1.1 Tablet Manufacturing

**4.1.1.1 Market Dominance:** The most common solid dosage form used in medication administration is the tablet.

**4.1.1.2 Process:** entails the compression or moulding of excipients and active pharmaceutical ingredients (APIs) into the appropriate shape.

**4.1.1.3 Excipients Role:** Control medication release, disintegration, and dissolution in accordance with patient requirements; lubricants and glideants are necessary for manufacturing facilitation.

#### 4.1.2 AI in Tablet Manufacturing

**4.1.2.1 Drug Release Prediction:** AI predicts systemic drug release.

**4.1.2.2 Process Optimization:** Investigates effects of crucial processing parameters, ensuring consistent quality control.

**4.1.2.3 Defect Identification:** AI applications identify defects in tablets, enhancing quality assurance.<sup>[46]</sup>

#### 4.2 Drug Release Prediction Using Formulations

Stable quality control depends on accurate medication release prediction. In vivo and in vitro drug release studies are basic technologies that are routinely assessed throughout the course of product development. Important material characteristics and manufacturing conditions affect how quickly the medication releases from oral solid dose forms. Compaction parameters (e.g., pressure for tablet hardness), tablet geometry, and drug loading characteristics are common variables influencing drug release. For lengthy drug release investigations, analytical approaches like spectrophotometric methods are frequently used. The formulator's specifications must be met, which means laborious and time-consuming repeated testing and batch preparation for optimisation are required.

By anticipating drug release and lowering the number of runs required to optimise batches, artificial intelligence (AI) helps in drug formulation by saving time and money on pilot scale and production operations. AI is able to analyse disintegration times, forecast drug release patterns, and choose the optimal batch for additional scaling. Researchers have predicted the

dissolving characteristics of hydrophilic matrix sustained-release tablets using artificial intelligence (AI) methods, such as artificial neural networks (ANNs). Regression analysis and support vector machines (SVM) are also used for data analysis and dissolution profile prediction.

Particle size distribution has been shown to be the most important variable during model prediction. Data for drug release modelling are generated utilising essential material properties and process analytical technology (PAT). As part of the assessment metrics<sup>[47,48]</sup>, ANNs are then utilised to determine which models are the most accurate.

#### **4.3 AI used in the 3D-Printed Dosage Forms**

Artificial Intelligence (AI) is transforming the pharmaceutical manufacturing industry by facilitating customised medication and optimising drug delivery via 3D printing. AI systems enhance medication therapy by optimising design and formulation in light of patient-specific parameters. Drug release patterns, strengths, and geometries may be quickly prototyped and optimised through the use of machine learning and computational modelling, which simulate behaviour. AI maintains quality control, optimises printing settings, and anticipates and resolves production difficulties. By learning from real-time data, feedback systems improve accuracy and scalability, improving patient outcomes and personalised therapy.

#### **4.4 AI Used for the Detection of Tablet Defects**

AI automates the identification of tablet flaws, revolutionising quality control in the pharmaceutical manufacturing industry. Tablet photos are analysed using AI algorithms and computer vision methods to find fractures, chips, discolouration, and size and form differences. When it comes to defect identification, AI models that have been trained on huge datasets outperform time-consuming traditional approaches like X-ray computed tomography in terms of precision and recall. X-ray tomography and deep learning together improve the precision of fault identification. Ma et al. improved accuracy and efficiency by analysing tablet flaws using neural networks, such as UNet models. AI-powered defect identification ensures prompt fault intervention, preserves product quality and safety, and minimises mistakes and subjective judgement by reducing reliance on manual inspection.<sup>[49,50]</sup>

#### **4.5 AI Used in Nanomedicine**

You seem to be highlighting how AI is revolutionising nanomedicine, especially in terms of creating nanoparticles, improving medication delivery methods, and forecasting how they will

behave in biological systems. Through real-time monitoring and feedback systems, this capacity not only improves medication efficacy and safety but also allows for personalised treatment methods. AI also helps to make nanocarrier creation more efficient and scalable, which is important for targeted therapies like the treatment of cancer. The understanding and creation of nanocarriers is further enhanced by the combination of AI with experimental approaches such as molecular dynamics and Monte Carlo simulations. These developments are essential to the development of nanomedicine towards more individualized and efficient medical treatments.<sup>[51,52]</sup>

#### **4.6 AI Application for Parenteral, Transdermal and Mucosal Route Products**

AI plays a crucial role in developing and manufacturing injectables, biologics, and complex pharmaceutical formulations by optimizing physicochemical parameters like pH, solubility, stability, and viscosity. It improves product quality, efficiency, and regulatory compliance through real-time data analysis and predictive modeling. AI enhances inspection processes using advanced algorithms for particle tracking and image processing, ensuring product quality and safety. Machine learning (ML) further accelerates drug delivery technology development by predicting drug release and optimizing formulation processes. Computational pharmaceutics, including multiscale simulations and *in silico* modeling, revolutionizes drug formulation design, advancing towards more efficient and precise pharmaceutical production in the era of Pharma 4.0.<sup>[53, 54, 55]</sup>

#### **4.7 AI Used in Medical Devices**

By improving diagnostics through the analysis of imaging data such as CT scans and X-rays, enabling remote health monitoring for chronic conditions, integrating into wearable devices for continuous health tracking, improving prosthetics for natural movement, aiding in precise surgeries, and efficiently managing medications, artificial intelligence (AI) has revolutionized medical devices. For example, Medtronic uses artificial intelligence (AI) in the Sugar IQ app and Guardian Connect system to give individualized support and real-time insights for managing diabetes. It also analyses glucose trends, provides glycemic assistance, and helps with dietary decisions for improved disease control.<sup>[56-57]</sup>

### **5. AI used In Pharmacokinetics and pharmacodynamics**

Pharmacokinetics and pharmacodynamics (PKPD) are crucial in defining dose, administration, and safety profiles during the complicated stages of drug development, which span from discovery to regulatory approval. Conventional approaches, such as research on animals and



clinical trials, are expensive, time-consuming, and may not accurately anticipate human reactions. These constraints are overcome by computational models and AI, which provide a quicker and more affordable solution by more precisely predicting PKPD. Despite difficulties with the amount and trustworthiness of data, AI integration, by utilising strong computing and machine learning techniques, improves predictions and optimisations in drug development.<sup>[58]</sup>

## 6. Limitations of AI Tools

**6.1 Data Dependency:** They require large amounts of high-quality data for training, which may not always be available or representative.

**6.2 Interpretability:** AI models can be complex and lack transparency, making it challenging to understand how they arrive at decisions.

**6.3 Bias:** Models can inherit biases from training data, leading to unfair or inaccurate outcomes, especially in healthcare and other critical domains.

**6.4 Ethical Concerns:** Issues like privacy, consent, and accountability arise when AI is used for sensitive tasks like diagnosis or decision-making.

**6.5 Robustness:** AI systems may struggle with unexpected inputs or scenarios outside their training data, affecting reliability in real-world applications.

## 7. Futuristic Overview of AI

**7.1 Personalized Formulations:** AI will enable the creation of personalized medicines tailored to individual patient profiles, optimizing efficacy and minimizing side effects.

**7.2 Predictive Modeling:** Advanced AI algorithms will predict complex physicochemical properties and behaviors of formulations, accelerating development timelines and reducing costs.

**7.3 Integrated Design Platforms:** AI-driven platforms will integrate data from various sources (genomic, clinical, and environmental) to design formulations that consider multifaceted patient factors.

**7.4 Real-Time Optimization:** AI systems will continuously optimize formulations based on real-time data feedback from manufacturing processes and patient outcomes.

**7.5 Multiscale Simulations:** Enhanced computational power will support multiscale simulations, simulating molecular interactions to design more precise and effective drug delivery systems.

**7.6 Regulatory Compliance:** AI will streamline regulatory compliance by analyzing vast datasets to ensure formulations meet safety and efficacy standards globally.

**7.7 Collaborative AI-Human Interaction:** AI will facilitate collaborative environments where human expertise and AI capabilities synergize, fostering innovation and rapid advancements in formulation science.

**7.8 AI in Quality Control:** AI-powered systems will enhance quality control by identifying deviations and optimizing manufacturing processes to ensure consistent product quality.

**7.9 Emerging Technologies:** Incorporation of AI with emerging technologies like nanotechnology and biotechnology will open new avenues for developing novel formulations with enhanced therapeutic capabilities.

**7.10 Environmental Impact:** AI will contribute to sustainable formulation development by optimizing processes to reduce waste and energy consumption, aligning with global sustainability goals.<sup>[59,60]</sup>

## 8. CONCLUSION

By utilising data analysis, pattern recognition, and optimisation, artificial intelligence (AI) is transforming medication delivery systems and allowing personalised, adaptive, and targeted medicines. Artificial intelligence (AI) techniques in pharmacokinetics and pharmacodynamics minimise the need for animal and human trials by predicting parameters, simulating drug distribution, and optimising doses. In the pharmaceutical industry's journey towards this era, computational pharmaceutics using AI and big data improves manufacturing efficiency, personalised medicines, formulation optimisation, regulatory compliance, and manufacturing efficiency. This holds the promise of quicker drug discovery and better patient outcomes.

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