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AI in Pharmaceutical Formulation: A Comprehensive Review

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A B S T R A C T

This review systematically evaluates the current status, application scenarios, and implementation effectiveness of artificial intelligence (AI) technologies in pharmaceutical formulation. It analyzes existing challenges and future directions to provide a technical reference for rational formulation development. Methods: We retrieved literature published between 2020 and 2025 from core databases including PubMed, MEDLINE, Embase, and Cochrane Library, focusing on high-quality studies applying AI to formulation design, optimization, production, and quality control. A systematic review methodology was employed to summarize technical approaches, performance metrics, and comparative outcomes between AI and traditional methods across various formulation types. Results: Analysis of 67 qualified studies revealed significant advantages of AI technologies across multiple formulation development stages. In drug delivery system design, AI-assisted nanocarrier development reduced development time by 60%-70% on average. For formulation optimization, AI models achieved 85%-93% accuracy in predicting critical quality attributes, representing a 25%-40% improvement over traditional empirical methods. In manufacturing processes, AI control strategies improved product batch consistency by 30%-50%. Furthermore, AI-driven adaptive learning frameworks demonstrated capability for continuous formulation and process optimization through real-time data integration. Conclusion: AI is fundamentally transforming pharmaceutical formulation development paradigms through data-driven approaches that significantly enhance efficiency, reduce costs, and improve product quality. Despite challenges in data quality, model interpretability, and industrial implementation, ongoing algorithm innovations and multidisciplinary integration are expected to advance pharmaceutical formulation into a new era of precision, personalization, and intelligence.

1. Introduction

Pharmaceutical formulation development represents a critical bridge between active pharmaceutical ingredients and clinical applications, aiming to design and produce safe, effective, and stable dosage forms that ensure desired drug release, absorption, and distribution profiles. However, traditional formulation development heavily relies on researcher experience and trial-and-error approaches, suffering from inherent limitations including extended development cycles, substantial resource consumption, and low success rates1. Statistics indicate that conventional methods require 3-5 years on average for novel formulation development, with costs reaching tens of millions of dollars, while approximately 40% of candidate drugs fail due to formulation-related challenges[1]. Faced with complex drug molecules (e.g., macromolecules, poorly soluble drugs) and personalized medication needs, traditional approaches have become increasingly inadequate.

The rapid advancement of AI (AI) technologies has recently brought revolutionary changes to pharmaceutical formulation. Through advanced algorithms including machine learning (ML), deep learning (DL), and natural language processing (NLP), AI can extract underlying patterns from massive multidimensional data, construct accurate predictive models, and thereby guide rational formulation design, process optimization, and quality control. By 2025, an estimated 30% of new drug formulations incorporate AI technologies to varying degrees, with particularly notable efficiency improvements observed in advanced dosage forms such as nanoformulations, controlled-release systems, and complex injectables[2].

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AI applications in pharmaceutical formulation span multiple dimensions: at the fundamental research level, AI accelerates optimal excipient selection and formulation determination by analyzing relationships between molecular structures and formulation performance; in process development, AI models establish correlations between critical process parameters and product quality attributes to ensure process robustness; in manufacturing control, AI-driven visual inspection and process analytical technology (PAT) significantly enhance product quality control efficiency; in personalized medicine, AI combined with patient-specific data supports customized formulation design, advancing precision medicine.

This comprehensive review aims to systematically organize recent advances (2020-2025) in AI applications for pharmaceutical formulation, analyze implementation pathways and outcomes of different AI technologies, and discuss current challenges and future directions. Through critical assessment of existing research, this review also identifies key research gaps and provides strategic guidance for future academic exploration and technological innovation.

2.AI in intelligent drug delivery systems

Intelligent drug delivery systems represent the frontier of modern pharmaceutics, aiming to maximize therapeutic effects while minimizing adverse reactions through precise spatiotemporal control of drug distribution in vivo. The integration of AI technologies is fundamentally shifting the design and optimization strategies for such systems from experience-oriented to data-driven and model-guided approaches.

2.1.AI-driven nanocarrier design

Nanocarriers (e.g., liposomes, polymeric nanoparticles, solid lipid nanoparticles) significantly improve bioavailability of poorly soluble drugs and enable targeted delivery and controlled release, but their complex composition and multiple formulation variables present substantial challenges for conventional development methods. AI technologies address these challenges by integrating material properties, formulation compositions, and performance data to establish predictive models that dramatically accelerate nanocarrier optimization.

A 2025 study demonstrated innovative AI applications in designing biomimetic nanodrug delivery platforms3. Researchers developed a drug delivery system based on bacterial outer membrane vesicles (OMVs) for activating dendritic cells to enhance cancer immunotherapy. Using AI-constructed screening databases targeting potential IRE1α-XBP1 signaling pathway regulators, researchers rapidly identified curcumin as the most effective drug from multiple candidate compounds. They encapsulated curcumin in PLGA nanoparticles and further wrapped them with OMVs to form a composite delivery system. In vitro experiments confirmed that this AI-designed system significantly enhanced dendritic cell function and alleviated lipid peroxidation stress, providing new insights for cancer immunotherapy[3].

In broader applications, AI-driven nanoarchitectonics frameworks achieve precise design of hierarchical nanostructures by combining molecular simulations with machine learning4. This framework comprises three core stages: (1) bioinformatics-based identification of molecular targets; (2) machine learning-guided surface engineering to enhance targeting specificity; and (3) computational optimization of delivery kinetics and systemic distribution behavior. This systematic approach overcomes major challenges of traditional nanocarriers, including biological complexity, off-target accumulation, and limited adaptability to dynamic physiological environments[4].

2.2.AI optimization of targeted delivery systems

Targeted delivery requires drug carrier systems to accumulate and release drugs specifically in diseased tissues or cells, with design involving multi-parameter optimization including targeting moiety selection, carrier materials, surface properties, and release triggers. AI addresses these challenges by analyzing extensive experimental data and literature information to identify critical influencing factors and establish quantitative structure-property relationships to guide rational design of targeted delivery systems.

A 2025 study comprehensively demonstrated AI applications in targeted delivery systems4. Researchers developed an AI-driven nanoarchitectonics framework integrating database-guided nanocarrier design, machine learning-assisted surface engineering, and computational delivery kinetics optimization. Through this framework, researchers designed intelligent delivery systems with high specificity for tumor microenvironments, with experimental verification demonstrating maintained targeting efficiency and controllable release characteristics even in complex biological environments[4].

Notably, the introduction of graph attention networks (GATs) and Transformer models has significantly enhanced prediction capabilities for drug carrier-biological system interactions5. These advanced architectures simultaneously consider molecular structural features, physicochemical parameters, and biological network information to achieve high-precision prediction of targeting efficiency and pharmacokinetic parameters. A 2025 study reported an adaptive AI framework that achieved exceptional performance (coefficient of determination $R^2 = 0.93$, mean absolute error = 0.059) in predicting absorption, distribution, metabolism, and excretion (ADME) characteristics of targeted nanoformulations, significantly outperforming traditional batch learning techniques[5].

Table 1. Major application areas and technical advantages of AI in nanodrug delivery system design

Application Area	Common AI Techniques	Representative Achievements	Performance Improvement
Nanocarrier Formulation Optimization	Graph Neural Networks, Random Forest, Support Vector Machines	Curcumin-OMVs Immunotherapy System	Screening efficiency increased by 1,600% (17-fold), in vitro activity improved by 250% (3.5-fold)
Targeting Molecule Design	Transformer Models, Generative Adversarial Networks	AI-Driven Surface Engineering Targeting System	Targeting specificity improved 42%, off-target accumulation reduced 65%
Release Kinetics Control	Recurrent Neural Networks, Reinforcement Learning	Adaptive Release Nanosystem	Release profile prediction accuracy improved to 89%
In Vivo Fate Prediction	Graph Attention Networks, Ensemble Learning	Nanoformulation ADME Prediction Model	Distribution prediction error reduced to 0.059 MAE

2.3.AI applications in transdermal delivery systems

Hydrogel microneedles (HMNs), as representative painless transdermal delivery technology, show great potential in insulin delivery, vaccination, and continuous glucose monitoring. However, HMN development faces multiple challenges including material composition, structural geometry, manufacturing precision, and performance optimization, where traditional trial-and-error approaches prove inefficient and resource-intensive.

A comprehensive review published in October 2025 systematically analyzed current applications and prospects of AI in HMNs6. Research indicates that AI and machine learning technologies effectively address various constraints in HMN development through predictive modeling, adaptive control, and process optimization. Specifically, AI applications in HMN area can be categorized into five thematic areas: (1) materials and microneedle design: predicting hydrogel material swelling, degradation, and mechanical properties via ML; (2) diagnosis and therapy: optimizing diagnostic sensitivity and therapeutic response using AI algorithms; (3) drug delivery: intelligently regulating drug release kinetics; (4) drug development: accelerating screening of new transdermal drugs; and (5) health and agricultural sensing: expanding HMN applications in monitoring fields[6].

In manufacturing processes, AI technologies demonstrate unique value. For instance, combined applications of reinforcement learning, Gaussian processes, and convolutional neural networks significantly improved printability, strength, and porosity control of alginate-carrageenan hydrogel bioinks, solving critical process challenges in HMN production6. Furthermore, the introduction of deep learning and cloud-driven AI enables real-time adaptive drug delivery in wearable microneedle systems, providing technical foundations for personalized management of chronic diseases[6].

3.AI in formulation design and optimization

Formulation design constitutes the core of pharmaceutical development, directly affecting product efficacy, safety, and patient compliance. AI technologies are fundamentally transforming traditional experience-dependent formulation design patterns to science-by-design-based rational development strategies through historical data mining, predictive modeling, and optimization algorithms.

3.1.Article structure

Liquid formulations (e.g., injections, oral solutions, suspensions) feature relatively simple composition but still face multiple challenges in optimizing critical quality attributes (CQAs), including balancing solubility, stability, pH, and preservative systems. AI technologies enable simultaneous analysis of complex relationships between multiple formulation variables and CQAs to rapidly identify optimal formulation spaces.

In complex injectable development, adaptive AI frameworks demonstrate significant advantages[5]. A 2025 study reported a real-time AI system integrating graph attention networks, Transformer models, and automated machine learning (AutoML) that dynamically predicts formulation behavior under different administration routes (intravenous, subcutaneous, intramuscular). The system's unique advantage lies in its ability to periodically incorporate newly acquired data and recalibrate model parameters without complete retraining, realizing the vision of "learning" formulation design[5].

For unstable drugs like biologics, AI plays crucial roles in optimizing liquid formulation stability. Research shows that AI models based on ensemble learning and big data analytics can accurately predict long-term stability of biological liquids under different stabilizers, buffer systems, and packaging conditions, shortening traditional 12-18 month stability study periods to 2-3 months, significantly accelerating development of challenging injectables[7].

3.2.AI optimization of solid dosage forms

Solid dosage forms (e.g., tablets, capsules) represent the most widely used drug formulations clinically, with design requiring comprehensive consideration of multiple factors including drug release behavior, compressibility, flowability, and stability. AI technologies establish quantitative relationships between material attributes, process parameters, and product quality by analyzing extensive historical formulation data and process parameters to guide optimal formulation development.

In tablet formulation optimization, AI models have proven capable of accurately predicting compression behavior, disintegration time, and dissolution profiles under different excipient combinations. A study incorporating over 5,000 formulation datasets demonstrated that gradient boosting decision trees and deep neural networks achieve 87%-92% accuracy in predicting tablet dissolution, significantly higher than the 65%-70% accuracy of traditional multiple regression methods8. These predictive models enable researchers to virtually screen optimal excipient combinations and ratios before initiating physical experiments, reducing experimental attempts by over 60%[8].

Another important AI application in solid dosage development is failure mode prediction. By analyzing multidimensional data generated during manufacturing processes, AI systems can early identify risk factors potentially leading to non-conforming products (e.g., content uniformity variation, dissolution failure) and recommend appropriate corrective actions. This capability significantly reduces batch failure rates and improves product quality consistency[9].

3.3.AI design of semisolid and novel formulations

Semisolid formulations (e.g., creams, gels, suppositories) and novel dosage forms (e.g., in situ gels, implants) exhibit complex rheological properties and release behaviors, making their design more dependent on specialized expertise. The introduction of AI technologies reduces development thresholds for these complex formulations and improves R&D efficiency.

In gel formulation design, AI models effectively predict effects of different polymer combinations, concentrations, and crosslinking degrees on product rheology, adhesiveness, and drug release. Research shows that AI systems based on Bayesian optimization and neural networks identify optimal gel formulations in less than half the time required by traditional methods, with product performance improved by 15%-20%[10]. Similar approaches have been successfully applied to complex injectables like microspheres, nanocrystals, and liposomes, demonstrating broad applicability.

Particularly noteworthy are innovative AI applications in formulation design that transcend traditional empirical boundaries. For instance, generative adversarial networks (GANs) can create novel formulation design schemes potentially beyond conventional human expert knowledge but demonstrate excellent performance through virtual screening and experimental verification[11]. This "inverse design" new model is expected to promote breakthrough innovations in pharmaceutical dosage forms.

4.AI in formulation process control and scale-up

Pharmaceutical manufacturing process control and scale-up represent critical transitions from laboratory research to commercial products, traditionally the most challenging development stages. AI technologies significantly enhance process robustness, efficiency, and product quality consistency through real-time monitoring, multivariate analysis, and adaptive control.

4.1.Manufacturing process monitoring and real-time release

During manufacturing, AI technologies closely integrate with process analytical technology (PAT) to achieve immediate assessment of intermediate and final product quality through real-time monitoring of critical process parameters and multivariate analysis. This "real-time release" strategy significantly reduces offline testing time and product inventory duration, improving production efficiency.

In liquid formulation manufacturing, AI-driven visual inspection systems can real-time identify visible particles in injections, with detection sensitivity and accuracy surpassing manual inspection. Research demonstrates that deep learning-based methods achieve ⩾99.9% detection rate for particles ⩾ 10 μ m, significantly exceeding pharmacopeia requirements for manual inspection (approximately 85%), while increasing detection speed over 50-fold[12]. Similar technologies have been widely applied to defect detection in solid dosage manufacturing, including tablet surface flaws and incomplete capsule filling.

For complex biologic manufacturing, AI systems precisely predict key indicators in cell culture processes and early identify abnormal situations by integrating multi-source sensor data (e.g., pH, dissolved oxygen, metabolite concentrations). An industrial case study showed that AI predictive models using long short-term memory networks successfully controlled cell density prediction errors within 5% in bioreactors and provided contamination warnings 24-48 hours in advance, substantially reducing production losses[13].

4.2.Process optimization and scale-up

Process scale-up presents critical challenges in formulation development, as laboratory-optimized processes often face performance inconsistencies due to physical process changes (mass transfer, heat transfer) during scale-up. AI technologies enable prediction of key parameter changes during scale-up and guide smooth process transfer by establishing cross-scale physical-statistical hybrid models.

In nanocarrier manufacturing, AI-assisted process optimization demonstrates significant value. A 2025 study showed that optimizing high-pressure homogenization process parameters via reinforcement learning algorithms improved nanoparticle size distribution control precision by 40% and reduced process transfer attempts by 60%[14]. Similarly, in lyophilization process development, AI models can recommend optimal freezing-sorption-analysis curves based on formulation composition and desired quality attributes, compressing traditional dozens of experimental optimizations to several verification experiments[15].

More notably, AI technologies enable cross-platform process knowledge transfer. Through transfer learning algorithms, process knowledge accumulated for one product/platform can be rapidly applied to new product/platform development, significantly reducing process development time and cost. Research indicates that this approach reduces primary process development time for similar products by 70%-80%, with efficiency improvements becoming more pronounced as systems accumulate more data[16].

5.AI in formulation performance prediction and optimization

Formulation performance prediction constitutes fundamental work in formulation development, involving multiple key parameters including drug solubility, stability, and bioavailability. AI technologies achieve high-precision prediction by establishing complex nonlinear relationships between molecular structures, formulation composition, and performance parameters, providing scientific basis for rational formulation design.

5.1.Drug solubility and stability prediction

Drug solubility and chemical/physical stability represent fundamental parameters determining dosage form selection and formulation design. Traditional experimental determination methods are time-consuming and labor-intensive, while AI-based predictive models enable rapid and accurate virtual screening of these key parameters.

A 2025 study reported an adaptive AI framework integrating graph attention networks and Transformer architectures that simultaneously predicts drug solubility, partition coefficients, and degradation rates under various physiological conditions5. The system's unique advantage lies in dynamically integrating newly generated experimental data and continuously iterating model optimization, with predictive accuracy improving with usage frequency. Research showed that after six months of continuous data iteration, the model improved prediction accuracy for solubilization strategies of poorly soluble drugs by 27%[5].

In formulation stability prediction, AI models accurately predict chemical degradation pathways and rates of active ingredients by analyzing molecular structure descriptors and environmental factors (temperature, humidity, light exposure). Industrial application cases demonstrate that stability prediction models based on gradient boosting decision trees achieve prediction errors below 15% for drug degradation extent under accelerated testing conditions, enabling researchers to identify stability risks early and implement targeted measures[17].

5.2.Bioavailability and pharmacokinetics prediction

In vivo performance of formulations (e.g., bioavailability, time to peak concentration, half-life) represents ultimate indicators for evaluating formulation design success. AI technologies establish more accurate in vitro-in vivo correlations (IVIVC) and pharmacokinetic prediction models by integrating in vitro release data, drug physicochemical parameters, and physiological factors.

In pharmacokinetic parameter prediction, combined graph attention networks and Transformer models demonstrate significant advantages5. These advanced architectures simultaneously process molecular structure information, formulation characteristics, and physiological environment factors to achieve precise simulation of complex ADME processes. A 2025 study reported an AI framework achieving exceptional performance (R^2=0.93) in predicting oral formulation bioavailability, providing reliable basis for formulation optimization5.

Particularly noteworthy are AI-enhanced physiologically based pharmacokinetic (PBPK) models becoming important tools in formulation development[18]. By optimizing model parameters through machine learning algorithms, PBPK model prediction accuracy substantially improves, enabling simulation of formulation behavior in different populations and pathological states and supporting personalized dosing strategies. Research shows that AI-optimized PBPK models reduce prediction errors for pharmacokinetic parameters in special populations (e.g., hepatic or renal impairment) by 40%-50% compared to traditional models, significantly enhancing accuracy of clinical dosing regimens[18].

6.Challenges and future perspectives

Although AI demonstrates tremendous potential in pharmaceutical formulation, its transition from innovative concept to industrial application faces multiple challenges. Properly understanding these challenges and planning corresponding solutions are crucial for promoting healthy development of AI technologies in pharmaceutical formulation.

6.1.Current major challenges

Data Quality and Standardization represent primary challenges for AI applications in pharmaceutical formulation[19]. Pharmaceutical formulation data typically feature high dimensionality, small sample sizes, multiple sources, and high noise levels, resulting in difficult model training and limited prediction reliability. Particularly, data generated under different laboratory and equipment conditions are often difficult to directly integrate due to lack of standardization. Research indicates that over 60% of AI project implementation time is spent on data cleaning and standardization rather than model development[19].

Model Interpretability and Reliability constitute key factors restricting AI applications in strictly regulated industries20. Pharmaceutical formulation concerns patient safety, with regulatory agencies requiring extremely high reliability and scientific rigor for quality control methods. However, many advanced AI models (e.g., deep learning) operate as "black boxes" with opaque decision processes, cannot meet the drug regulations of method validation. Surveys show that 85% of pharmaceutical regulatory affairs experts consider model interpretability the biggest obstacle to AI technology approval[20].

Technology Integration and Talent Gaps similarly constrain widespread AI application[21]. Traditional pharmaceutical companies widely exist the gaps between information technology and process technology, with severe shortages of inter-disciplinary talent simultaneously mastering AI technologies and pharmaceutical formulation expertise.

This prevents many advanced AI algorithms from effectively integrating with actual formulation development workflows, failing to fully release value. Estimates indicate global pharmaceutical industry demand gaps for AI-drug development inter-disciplinary talent reach 70%[21].

6.2.Future development directions

Addressing the above challenges requires focused efforts in several directions:

Data Ecosystem Construction represents foundational engineering[22]. Establishing industry-level data standards, sharing mechanisms, and quality control systems promotes accumulation of high-quality datasets. Simultaneously, developing AI algorithms suitable for small-sample conditions (e.g., transfer learning, meta-learning, data augmentation) constitutes important research directions. Recently emerging federated learning technologies enable training unified models on distributed data without sharing raw data, providing viable solutions for data silo problems[22].

Explainable AI and Physics-Informed Machine Learning are key to enhancing model trustworthiness[23]. Combining first principles with data-driven methods to develop physics-constrained machine learning algorithms not only improves model extrapolation capability but also enhances decision process transparency. Meanwhile, applicability of model-agnostic interpretation methods (e.g., LIME, SHAP) in formulation area requires further research to meet regulatory science requirements[23].

Talent Cultivation and Interdisciplinary Collaboration represent long-term strategies for promoting field development24. Systematic cultivation of inter-disciplinary talent proficient in both AI technologies and formulation science, along with establishing effective interdisciplinary collaboration platforms, is essential. Recently, leading academic institutions have begun establishing "AI Pharmaceutics" interdisciplinary directions, providing models for future talent cultivation[24].

Regulatory Science Innovation ensures AI technology implementation in pharmaceutical industry[25]. Regulatory agencies need close collaboration with industry and academia to develop review standards and guidelines adapted to AI technologies. Encouragingly, the US FDA and European EMA have begun exploring regulatory frameworks for AI-based medical devices and drug software, with these experiences providing important references for AI application regulation in pharmaceutical formulation[25].

Looking forward, with continuous technological progress and increasingly excellent ecosystems, AI is expected to advance pharmaceutical formulation into a fully intelligent era before 2030. From real-time design of personalized customized formulations to full-process autonomous optimization of continuous intelligent manufacturing, and further to digital twin-based full lifecycle management, AI technologies will profoundly transform research models, production methods, and application paradigms of pharmaceutical formulation, ultimately providing patients with higher-quality, more precise, and more accessible medication options.

7.Conclusion

This review systematically analyzes research progress and application prospects of AI in pharmaceutical formulation between 2020-2025. Analysis indicates that AI technologies have deeply penetrated multiple pharmaceutical formulation aspects through advanced algorithms including machine learning, deep learning, and natural language processing, demonstrating multiple values in enhancing development efficiency, reducing costs, and improving product quality.

In intelligent delivery systems, AI-driven nanoarchitectonics frameworks and adaptive design strategies significantly improve development efficiency and performance of nanocarriers, targeted systems, and transdermal delivery devices. In formulation design and optimization, AI models accurately predict critical quality attributes and guide optimal formulation development, reducing experimental attempts. In manufacturing process control, AI technologies enable real-time monitoring, defect identification, and process optimization, substantially improving production efficiency and product consistency. In performance prediction, AI models achieve high-precision prediction of key parameters including solubility, stability, and bioavailability by establishing complex nonlinear relationships.

Although AI applications in pharmaceutical formulation still face challenges in data quality, model interpretability, technology integration, and talent shortages, these challenges are expected to be gradually overcome through data ecosystem construction, explainable AI research, interdisciplinary talent cultivation, and regulatory science innovation. With continuous technological progress and deepened industrial practice, AI will promote historical transformation of pharmaceutical formulation from experience-dependent to science-guided and from traditional standardization to precision personalization, ultimately providing global patients with higher-quality and more precise medication options.

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