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Current trends in the use of Artificial Intelligence in the Development of Pharmaceutical Formulations

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Abstract

The development of pharmaceutical formulations is an empirical, resource-consuming and trial-and-error driven process. With the advent of the Fourth Industrial Revolution (Industry 4.0), artificial intelligence (AI) and machine learning (ML) have emerged as disruptive paradigms that can revolutionise formulation science into an explicit, data-driven, and predictive discipline. The comprehensive review discusses the mechanism and technology architectural layers of AI integration such as artificial neural networks, support vector machines, random forests, fuzzy logic and deep generative structures. We group the broad formulation domains under active optimisation, which encompasses immediate and modified release systems, lipid-based architectures, and complex biologics. Moreover, the review details the fundamental optimisation of preparation methodologies such as direct compression, hot-melt extrusion, 3D printing, and microfluidics through predictive workflows. Computational soft sensors are used to systematically evaluate evaluation parameters from critical quality attributes (dissolution profiles and compaction kinetics) to long-term stability. In this paper, recent state-of-the-art advances up to 2026 are summarised, including operational advantages, intrinsic mathematical limitations and regulatory hurdles. Finally, we discuss recent advanceents such as autonomous self-learning laboratories, digital twins, and continuous closed-loop molecular manufacturing, providing a holistic roadmap for modern pharmaceutical scientists.

Keywords: AI, Artificial Intelligence, Machine Learning, Pharmaceutical Formulation, QbD, Predictive Modelling

Introduction

The conventional method of formulation development in pharmaceutical field heavily relies on a sequence of empirical experimentations (Mak and Pichika). On the other hand, people who make medicines have to deal with a lot of different things. There are dozens of possible active ingredients, hundreds of other things that can be added to make the medicine, and lots of ways to make it (Das et al.). Previously, all this was done through trail and error method or through traditional design of experiments (DoE) methods (Paul et al.). While traditional methods shows multiple ways of collecting and analysing data, it often fails to deal with the complex, multi- part that are common in modern drug delivery systems (Fleming). These limitaions in the conventional methods often leads to longer time in product development, higher research and development costs and also the products are not at their highest quality (Moingeon et al.).

In recent years, particularly between 2020 and 2026, the pharmaceutical industry has seen a lot of change in how it uses artificial intelligence and machine learning (Swinney and Anthony; Yang et al.). Use of computer applications can be used to explore historical datasets to understand how complex structures and properties are interconnected without having to do practical experiments (Nelson et al.). Artificial Intelligence can handle large amount of data, including information of chemicals, particle size, heat levels and spectroscopic signatures to improve the result output (Piroozmand et al.; Harrer et al.). This shift from being reactive and testing-heavy to using simulations to predict how things will work also aligns perfectly with the regulatory requirements for Quality by Design (QbD) and real-time release testing (RTRT) within Industry 4.0 (Kolluri et al.; Warke et al.). This review shows how AI is used in pharmaceutical formulation, including mechanisms, classification strategies, preparation advancements, and evaluation frameworks utilising AI, concluding with an analysis of recent breakthroughs and the horizon of autonomous laboratories

Mechanism

The most important part of using AI in pharmaceutical formulation is mapping, it includes input variables like amount of different ingredients, mixing time, compaction force etc, onto target responses like tablet hardness, dissolution rate, disintegration time and chemical stability (Joshi and Sheth). Also using advanced ML architectures, we can build complex, multi-dimensional structures that can spot subtle synergistic or antagonistic interactions between the components in a formulation (Bermudez and Wolber). The main engine behind the artificial intelligence is the Artificial Neural Network (ANN) which works by simulating how our brain works by having multiple processing nodes that are all interconnected (Rani and Sharma). Different types of neural networks are used in different stages of the formulation development (Chaudhari and Patil; Garg and Verma).

In the field of machine learning, Support Vector Machines (SVMs) is used for structural risk minimisation to construct optimal hyperplanes for classification and regression tasks in high-dimensional spaces (Garg and Verma). Tree-based ensemble structures, especially Random Forests (RF) and Gradient Boosted Trees (GBT), work by combining the predictions made by multiple decision paths, which reduces the risk of data overfitting and effectively handles noisy data (Zhang and Tan; Mishra and Rahman). Natural Language Processing (NLP) text-mining pipelines extract information about how well different substances work together and toxicity profiles from unstructured regulatory files and historical scientific publications (Alves and Santos). Genetic Algorithms (GAs) are a type of computer program that are used for copying the way animals and plants evolve by selecting, combining, and changing its genes to achieve multiple goals at the same time (Chaudhari and Patil; Ahmad and Khan).

Types of AI Applications

AI applications used in pharmaceutical formulation can be classified based on their algorithmic intent and data structure. By understanding these different categories, researchers can easily choose the right tool based on their needs in various stages of the formulation development.

Generative and Reinforcement Architectures

Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs) are used to synthesise entirely new formulation combinations or simulate what might happen if a formulation were used, in cases where there is not enough data (Thomas and Moore). Reinforcement Learning (RL) agents are always learning, getting better at controlling the manufacturing process by trying and making mistakes in a virtual environment (Taylor and Brown; Davis and Wilson).

Supervised Predictive Modeling

Supervised frameworks are used for predictive analysis, where models acquire data from fully labelled historical datasets (Bordoloi et al.). These structures are divided into two types of tasks. The first type is continuous regression tasks which predicts the exact amount of drug released at different times an the second type is discrete classification tasks. These categorise excipient blends as either 'compactible' or 'non-compactible' (Silva and Costa). In this area, there are two types of model that are commonly used: multi-layer perceptrons (MLPs) and support vector regressions (Silva and Costa; Lee and Choi).

Unsupervised Pattern Recognition

In case of unlabelled multi -variate datasets, the use of unsupervised algorithims is used to facilitate the identification of latent structures and clusters (Wang & Liu). Principal Component Analysis (PCA) and t-Distributed Stochastic Neighbor Embedding (t-SNE) are used for transforming high dimensional data into visualisable mapping spaces (Taylor and Brown). Hierarchical and k-means clustering algorithms are used to identify alternative suppliers or alternative chemical entities that have the same mechanical properties (Roberts and Jones).

Preparation Methods and Process Optimization

The synthesis and mechanical strength of a pharmaceutical dosage form mainly depends on how they are processed. AI has shown promising results in eliminating manufacturing errors in case of complex preparation methods across multiple unit operations.

Direct Compression and Granulation

For manufacturing oral solid dosage form, direct compression method is the most efficient way to make them (White and Green). AI models have been developed to control the compressibility, compactibility and tabletability profile of powder beds. These models mainly works on the principle of true density, particle sizeand moisture levels of the raw materials (Harris). Controllers are used for continuous checking of binder spray rates, roller compaction and impeller speeds. In case of any changes needed in the setting to keep the granule size same, these changes are automatically made (Harris; Clark and Lewis).

Hot-Melt Extrusion and Amorphous Dispersions

HME is used to help the surface absorb molecules that does not dissolve well in the body (Walker and Hall). AI models uses datasets like the Hansen solubility parameters and the glass transition temperatures to predict how well drugs and polymers can be mixed together (Allen and Young). Deep learning models are also used to map the relation between extrusion temperatures, screw configurations and torque levels. These models mainly aims to prevent thermal degradation while ensuring complete amporphisation (King and Wright).

3D Printing and Microfluidics

When it comes to making personalised printlets, AI models can be used to control nozzle temperatures, printing speeds and infill percentages. This make sures of accurate mass uniformity and structural integrity (Patel and Shah; Scott and Adamson the other hand, in case of microfluidic manufacturing of lipid nanoparticles, machine learning models analyse continuous flow rates, Reynolds numbers, and total fluid flow rates in order to make sure that particle size are same at all time (Baker and Nelson).

Evaluation Parameters and Sensors

The evaluation of a pharmaceutical product includes the verification of a range of mechanical, physical, and chemical parameters. Previously, these assessments were conducted by using destructive, time-consuming, and offline methods. The utilisation of artificial intelligence facilitates the integration of 'soft sensors' that calculate these properties continuously by using non-destructive inline signalling methods.

In Vitro Dissolution and Release Profiles

Dissolution profiling is used to know how something actually works inside the body, it shows the in vivo behaviour of the body. Machine learning is used to predict drug release over time based on the structure of the polymer matrix (Carter and Mitchell). For example, the release rate can be modelled using automated variants of the Korsmeyer-Peppas equation:

$$Mt / M\infty = k \cdot tn$$

2

where k is the release structural constant and n is the transport exponent. These parameters are computed in real time by artificial intelligence (AI), which processes polymer viscosity, swelling indicators, and medium pH values (Evans and Turner).

Mechanical Properties and Compaction Kinetics

Friability, tensile strength and solid fraction metrics of a tablet are vital for industrial handling (Stewart and Morris). AI uses powder compaction energies and the Heckel equation constant to predict punch forces and avoid common manufacturing defects like capping, lamination, or sticking during high-speed production (Stewart and Morris; Inoue and Tanaka).

Accelerated stability and Predictive Shelf-Life

To figure out how stable chemicals and physical substances are usually means doing long-term experiments in an environmental chamber (Sato and Nakamura). Machine learning algorithms process short-term and high-stress degradation profiles (like high temperature and humidity variations) to predict long-term stability of chemical and polymorphic transitions up to 36 months out, saving a lot of time in development (Inoue and Tanaka; Lopez and Garcia).

Advantages and Limitations

Integration of Artificial Intelligence into formulation development offers significant advantages, although there are a few technical limitations.

Advantages

The main benefit of using AI in formulation development is that it can reduce the time to develop a new product, and also reduce the number of failed experiments (Carvalho and Ribeiro). AI can be used to check tens and thousands of virtual formulations on the computer, which helps in finding the best combinations of API and excipients much more quickly (Teixeira and Almeida). Moreover AI can also be used to find complex interaction parts of a drug that might be missed by the human researchers, which results in more effective and safer drugs (Vieira and Pinto).

Limitations

On the other hand, AI architectures are often subject to the well known “garbage in and garbage out” limitation (Mendes and Rocha). AI models highly depend on the availability of structured, high-quality, and standardised datasets (Barros and Fonseca). Machine learning setups works like a black box, which makes it hard to see how they works (Correia and Neves). This lack of transparency can cause problems during regulatory reviews (Correia and Neves). These platforms are costly to build and smaller generic manufacturers can barely afford them (Nunes and Soares; Gouveia and Marques).

Recent Advances

Recent developments up to 2026 has shifted the focus from individual property modelling to fully integrated, multi-system models. A key part of this is the use of Explainable AI (XAI) tools, such as SHapley Additive exPlanations (SHAP) and Local Interpretable Model-agnostic Explanations (LIME) (Thomas and Moore). These tools shows the detailed insights of how the formula and the process affect the final product's quality (Thomas and Moore). This improvement solves a big problem with the rules by making sure that the decisions made by the model can be checked and understood.

Another significant development is the integration of Active Learning loops with automated robotic workstations (Mendes and Rocha). In these configurations, an AI model guides a robotic system to prepare and analyse a small set of targeted formulations (Mendes and Rocha; Cardoso and Baptista). The system then uses the new data to improve the AI model, making it better at predicting things and creating more accurate virtual designs (Cardoso and Baptista). Also, large language models (LLMs) that are tuned for chemistry can now be used to automatically generate regulatory technical documents, compile batch data and stability metrics into perfect electronic data ready for agency submission (Antunes and Cunha; Fernandes and Couto).

Conclusion

Artificial intelligence to create new medicines is a big change from the old way of doing things. The old way was to test chemicals and change them until they worked well. Now we use data to ensure our medicines are safe and effective. The industry is tackling long-standing challenges in preformulation screening, excipient compatibility and complex process scaling with the use of advanced structures such as neural networks, tree ensembles and generative systems. There remain real issues around data standardisation, model transparency and regulatory pathways, but recent advances in explainable AI and automated active learning loops are making it much easier to move forward. With the advancement of technology, we are heading towards a future where computers assist in the discovery and production of pharmaceutical products. Artificial intelligence plays a big part in this. This change means that new treatments can be developed more quickly, to the same high standard each time, and adapted to meet the changing needs of patients around the world.

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