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ARTIFICIAL INTELLIGENCE IN DRUG DELIVERY SYSTEM DESIGN: FROM PREDICTIVE MODELING TO INVERSE FORMULATION DESIGN

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ABSTRACT

AI is revolutionising medication delivery research by enabling data-driven prediction, multidimensional formulation optimisation and rational design of delivery devices with increased therapeutic performance. Traditional drug delivery development is heavily dependent on iterative experimental approaches, empirical manipulation of formulations and step-wise optimisation of single formulation variables which are resource intensive and potentially inadequate to capture complex non-linear interactions between drugs, excipients, physicochemical characteristics, biological barriers and process parameters. Machine learning, deep learning, artificial neural networks and AI-based generative computational techniques offer possibilities to model these multidimensional interactions and to speed up the finding of formulations with defined performance features. Predictive modelling can be used to predict drug release kinetics, physico-chemical stability, pharmacokinetic behaviour, drug-excipient compatibility and carrier related properties to support early stage formulation decisions. AI-assisted optimisation enables systematic combination of formulation and process parameters to identify parameter combinations that result in good drug loading capacity, particle properties, encapsulation efficiency, stability and controlled or targeted release. More recently, a new paradigm was developed called inverse design approaches where the desired therapeutic/material features are first described and mathematical models then propose potential formulations that can achieve the predefined characteristics. Coupling generative AI with inverse design could further boost this capacity to build novel delivery structures outside the empirically investigated formulation space. However, there remain several challenges to be addressed, including data heterogeneity, limited datasets, model interpretability, external validation, reproducibility, regulatory approval, and the translation of computational predictions to clinically viable formulations. This review critically discusses the evolving role of AI in drug delivery with focus on forecasting, formulation optimisation and emerging inverse design strategies as well as translational barriers and future opportunities to develop more efficient, personalised and rationally engineered systems for drug delivery.

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1. INTRODUCTION

The efficient design of pharmaceutical delivery systems requires a multidisciplinary effort and the coordinated optimisation of drug physicochemical characteristics, carrier composition, formulation architecture, manufacturing circumstances, biological interactions, and therapeutic objectives. Despite significant developments in nanotechnology, biomaterials science, controlled release technologies, and targeted delivery, the innate complexity of formulation-performance interactions has impeded the translation of novel delivery platforms into clinically viable formulations. Rather than being determined by individual formulation variables, the transport of a drug is determined by complex and sometimes non-linear connections between drug properties, excipient properties, particle shape, surface properties, processing parameters, physiological conditions and biological barriers. Therefore traditional empirical development procedures based on repetitive experimentation could become resource heavy and not fully exploiting the multidimensional design space for advanced formulations [1,2]. The increasing availability of pharmacological, physicochemical, pharmacokinetic, biological and manufacturing datasets has presented a significant potential to augment experimental formulation development with artificial intelligence (AI)-based computational approaches. Machine learning (ML) and deep

learning (DL) approaches may recognise complicated patterns in multidimensional data sets and identify predictive correlations between formulation inputs and critical quality metrics. Recent accomplishments show the broader application of AI in drug formulation, design of nanocarriers, formulation characterisation and pharmaceutical optimisation, enabling a move from largely empirical development to a more data-driven formulation science [2,3]. ML models are beneficial in complicated drug delivery networks [1,3] as they can capture non-linear interactions and high dimensional feature spaces, unlike standard statistical approaches, which depend on a priori assumptions about the relationship between variables. Prediction modelling is one of the most important applications of AI in medication delivery research. Through computational modelling crucial formulation parameters including particle size, size distribution, surface characteristics, encapsulation efficiency, drug loading capacity, drug release behaviour, stability and other important quality attributes can be predicted. Recent research [2] shows that ML based techniques are being increasingly studied across polymeric nanoparticles, lipid nanoparticles, liposomes, nanoemulsions, nanocrystals and other nanoparticulate systems. Such predictability could be useful in picking formulation variables at an early stage, allowing investigators to concentrate on experimentally promising options before intense laboratory optimisation. Importantly, AI-based prediction should be seen as complementary to experimental study, as the reliability of models depends on the quality of the datasets, proper validation, concerns related to the applicability area and experimental confirmation [1,2]. AI based formulation optimisation is one step beyond prediction, to systematic decision assistance. Modern pharmaceutical formulations may contain a number of interacting variables such as polymer or lipid composition, surfactant concentration, drug to carrier ratio, solvent conditions, processing parameters and ambient conditions. Inefficient and fail to identify higher level links are the traditional one-factor-at-a-time approaches of optimising numerous variables simultaneously. ML-guided optimisation frameworks increasingly employ surrogate modelling, Bayesian optimisation, active learning and multi-objective optimisation approaches to explore complex formulation spaces with fewer wasted trial iterations [1]. Such methods are of particular importance when more than one formulation criterion must be fulfilled simultaneously, e.g. adequate particle properties, high encapsulation efficiency, controlled drug release, physical stability and acceptable manufacturability. Another conceptual development is inverse design, where first the desired properties for a delivery system are defined, and then a computational search for possible delivery system formulation compositions or process parameters is performed. This technique reverses the typical way of creating a formulation. Rather than selecting formulation inputs and measuring the resulting characteristics, the researcher determines the properties that he or she wants and calculations are used to determine what combinations of inputs can provide those properties. Recent work showed the move from trial-error formulation synthesis to AI assisted inverse design, combining predictive models with given medicinal and material targets [4]. This can be particularly useful for multifunctional nanocarriers, when the number of experimental designs available is far smaller than the theoretical formulation combinations. The paradigm can be further extended by generative AI which is capable of computationally generating new candidate materials and delivery architectures. Generative techniques can investigate complex chemical and material space and may give opportunities not easily found by conventional optimisation procedures [5]. But just because something is computationally unique doesn't mean it will be pharmacologically viable. Translation obstacles include data heterogeneity, small dataset size, model interpretability, external validation, repeatability, scalability, manufacturing constraints and regulatory approval [1,3,4]. In this context, this article analyses the rising application of AI in drug delivery, with a focus on the use of predictive modelling for formulation optimisation and the development of inverse design methodologies. The paper also covers the integration of ML, DL and generative computational techniques in pharmaceutical formulation research and provides a critical discussion on data limitations, model interpretability, experimental validation, regulatory considerations and future translational possibilities. This perspective is particularly essential when AI-assisted medication delivery transitions from computational proof-of-concept research to more integrated and experimentally supported formulation development workflows [1,4].

2. ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN DRUG DELIVERY SYSTEMS

Artificial intelligence (AI) has evolved as a computational framework that may potentially revolutionise the way in which drug delivery is produced from predominantly empirical trial to data-driven and mechanism-based design. Typically, formulation development proceeds on the basis of sequential testing where each formulation variable is altered independently and its effect on defined quality standards is empirically evaluated. There are several interacting components in delivery systems and the efficiency of distribution procedures decreases more and more. Formulation composition, processing circumstances, material properties and biological reactions may have nonlinear and strongly related relationships. Machine learning (ML) provides an alternative route: learning quantitative correlations from experimental data and utilising them to predict formulation behaviour over undiscovered parts of the design space [6,7]. Recent literature highlights that the primary use of AI in drug delivery is not to replace pharmaceutical expertise but to augment experimental reasoning by computationally uncovering complicated structure–property–performance links [6]. For this type of study, formulation descriptors can be correlated to the relevant quality attribute that is empirically obtained using supervised learning approaches such as random forest, support vector machine, artificial neural networks and Gaussian-process-based models. Deep learning can be advantageous in the case of high dimensional datasets and complex nonlinear interactions, however the effectiveness of deep learning mostly depends on the size, quality and standardisation of the dataset [8]. Thus, AI approaches have been developed to predict physicochemical and functional characteristics of polymeric nanoparticles, lipid nanoparticles, liposomes, nanocrystals, nanoemulsions and other new delivery systems [9]. Crucially, current developments are progressively merging

AI with high throughput experimentation, automation and adaptive learning to provide a framework in which computational predictions can guide subsequent experiments in a continuous manner [10]. AI thus provides a developing methodological bridge spanning pharmaceutical formulation research, materials informatics, computational modelling and experimental optimisation. In a broader sense, it allows formulation scientists to investigate increasingly complex design spaces, while keeping experimental validation at the core of pharmaceutical research.

3. PREDICTIVE MODELING AND DATA-DRIVEN PREDICTION OF DRUG DELIVERY PERFORMANCE

Predictive modelling is one of the most widely used uses of AI in medication delivery. It provides a computer platform to anticipate the behaviour of the formulation before any extensive experimental research is undertaken. Drug delivery mechanisms can be classified on the basis of a number of interdependent important quality criteria including particle size, polydispersity, surface charge, morphology, encapsulation efficiency, drug loading capacity, physical stability, dissolution behaviour and release kinetics. ML models are capable of learning quantitative links between these attributes and formulation or processing elements, such that delivery-system performance can be predicted given empirically collected input parameters [9, 11]. Recent studies and reviews highlight the need for such techniques, particularly for nanoparticulate systems, where small changes in composition or manufacturing circumstances can induce significant changes in physicochemical attributes and, consequently, impact biological performance. Predictive modelling can also be extended beyond physicochemical characterisation to biological and pharmacological effects. AI models can combine formulation properties with cellular absorption, permeability, biodistribution, toxicity, transfection efficiency or pharmacokinetic data sets to build more generic formulation-biological response linkages [11]. This inclusion is especially relevant in nanomedicine since superior physicochemical qualities do not necessarily mean appropriate therapeutic activities. Such prediction frameworks that integrate material properties and biological endpoints offer a more therapeutically relevant picture of delivery-system performance. Another citical application is the prediction of drug release behaviour. In classical release modelling empirically measured profiles are usually compared to pre-determined kinetic equations. In contrast, AI-based systems could learn the non-linear connections between formulation composition, material quality, ambient conditions and the release results. This may allow for the rapid identification of formulations that can achieve pre-defined temporal release profiles [6,12]. But prediction accuracy alone does not suffice to demonstrate pharmaceutical dependability. Heterogeneity of datasets, small sample numbers, experimental variance, imprecise specification of features and poor external validation can all severely limit model generalisability. Good data pre-processing, independent validation, computation of uncertainty and tested forecasts via experiments are therefore important for successful forecasting. Such needs are primarily identified as critical for the transition of AI-based prediction from proof-of-concept research to reproducible formulation development [7,11].

4. AI-DRIVEN FORMULATION OPTIMIZATION AND INTELLIGENT DESIGN OF DELIVERY SYSTEMS

AI-enabled formulation optimisation is not mostly about predicting formulation performance, but rather the computational identification of formulation situations that can achieve predefined quality objectives. Pharmaceutical formulations often consist of a number of interacting variables such as medication concentration, polymer or lipid composition, surfactant concentration, solvent ratio, processing temperature, mixing conditions and manufacturing parameters. Thus optimisation is a multi-dimensional challenge which has to take into account together formulation composition and process factors. Recent breakthroughs in ML-guided optimisation emphasise the promise of surrogate modelling, bayesian optimisation, active learning and multi-objective optimisation to explore such complicated design spaces with fewer trial iterations [6]. AI-assisted optimisation of nanoparticulate drug delivery has been used to discover the formulation conditions related with optimal particle size, polydispersity, encapsulation efficiency, drug loading, stability and release behaviour. This approach is especially applicable to lipid nanoparticles, polymeric nanoparticles, liposomes and other similar systems where the shape and function of the carrier is dependent on plurality of formulation components [9]. This can be further advanced by high-throughput experimental systems that provide standardised data sets for ML algorithms, enabling the learning of formulation-performance connections at scales many orders of magnitude higher [10]. One of the major breakthroughs is multi-objective optimisation, when artificial intelligence algorithms take into account multiple conflicting aims of pharmaceuticals concurrently, instead of focusing on a single parameter. For example, increasing drug loading can influence stability whereas particle size variation can influence cellular absorption and biodistribution. Therefore, AI based optimisation can uncover a set of formulations that show acceptable trade-offs between multiple essential quality criteria, rather than looking at each parameter in isolation [6]. Recent breakthroughs further exhibit integration of AI with Quality-by-Design ideas, automated experimentation, and closed-loop optimisation. In these systems, the experimental data are fed back into the computational model, the model updates its predictions and the next experiments are selected based on the information that is deemed to have the most value for optimisation. The iterative nature of the architecture drives the development of formulations toward an adaptive and self-improving approach. However, for its successful implementation, there is a need for good quality datasets, standardised experimental methodologies, interpretable models and empirically proven optimisation findings. Hence, AI-based formulation optimisation should be regarded as a smart decision support system that supplements, but does not replace, pharmacological experimentation.

5. EMERGING INVERSE DESIGN AND GENERATIVE AI STRATEGIES FOR NEXT-GENERATION DRUG DELIVERY

The notion of inverse design signifies a paradigm shift in the development of drug delivery, reversing the standard process of formulation engineering. In the traditional forward design, the process and formulation parameters are chosen first and the physicochemical or biological attributes are determined empirically later. Inverse design is a process that specifies the desired performance criteria first and then uses computer algorithms to identify conceptual designs predicted to meet those objectives. This is particularly useful in the case of sophisticated delivery systems where the number of alternative formulations can theoretically be far more than the number of formulations that can be physically synthesised and tested experimentally [13]. The advent of generative AI has notably expanded the conceptual area of inverse design. Generative models such as variationalautoencoders (VAEs), generative adversarial networks (GANs) and conditional versions thereof can be trained to acquire latent representations of material or formulation spaces and then produce candidate structures that satisfy the needed constraints. Recently, conditional generative neural networks have demonstrated their capability to generate multiple nanoparticle candidates for a given target property, illustrating how generative approaches can address the limitation of conventional predictive models that usually return a single output for a given input condition [14]. Generative AI has been researched for pharmaceutical formulation, enabling digital design and optimisation of dosage-form structures based on critical quality attributes. These trends suggest that the development of formulations may be shifting increasingly from experimental screening of current formulations to computational design of candidate systems that have not been previously synthesised [15]. The future role of inverse design will be its combination with predictive modelling, high throughput testing and automated synthesis. A closed loop technique can define a treatment goal, computationally generate candidate formulations, estimate physicochemical and biological performance, experimentally analyse the leading candidates and feed results back to the model. This approach can iteratively explore the design space and reduce needless experiments [10,13]. However, inverse design is still a nascent subject and not a commonly accepted approach for pharmaceutical development. The generated candidates are next synthesised, characterised, physiologically assessed and lastly verified translationally in an experimental setting. But there remain fundamental challenges: data deficiency, model uncertainty, chemistry / formulation feasibility, interpretability and regulatory acceptance. Yet this step from prediction to optimisation to goal-directed inverse design is one of the most notable accomplishments in AI-enabled medication delivery research.

6. FUTURE PERSPECTIVES

The future development of AI-enabled pharmaceutical delivery systems likely be marked by increased integration of mechanistic pharmaceutics, improved biomaterials, high-throughput testing, and patient-specific biological information with computational intelligence. The vision is that AI will evolve from a simple forecasting tool to a comprehensive decision-making tool that integrates molecular characteristics, formulation composition, manufacturing parameters, biological interactions and therapeutic outcomes during different stages of drug delivery development. This combination could allow the construction of computerised models of delivery systems that are refined iteratively with experimental and clinical data. The inverse design and generative AI will be at the forefront, which may allow for the design of formulations based on pre-determined medicinal and material aims rather than empirically selected mixes. Future models may improve simultaneously several parameters including drug loading capacity, release kinetics, physicochemical stability, tissue targeting, biocompatibility, manufacturing and scale-up. Integration with automated formulation platforms and robotic experimentation could take closed-loop processes further, where AI-generated candidates are experimentally synthesised, characterised and fed into subsequent computational learning cycles. Another important frontier is multi-modal data integration. Datasets of formulations can be combined with molecular frameworks, imaging data, pharmacokinetic profiles, omics data and patient-specific characteristics to enable more personalised delivery-system design. But to fulfil this promise, we need uniform datasets, interoperable data infrastructures, future validation, explainable models and rigorous approaches for assessing uncertainty. And rules need to keep up with expanding AI models, to assure reproducibility, traceability and patient safety. Finally, successful translation of AI into medication delivery will depend not only on the sophistication of the algorithms, but also on the degree to which computational predictions are integrated with pharmaceutical expertise, experimental data, quality-by-design principles and clinically important endpoints.

7. CONCLUSION

Computational approaches allow the assessment of complicated interactions in formulation, material, biological, and pharmacokinetic data sets, and AI is rapidly transforming the conceptual and methodological landscape of drug delivery development. Machine learning and deep learning techniques have proven promise in predicting critical formulation properties, drug release behaviour, physicochemical stability and aspects of biological performance, providing a rational basis for decreasing the need for substantial empirical study. Apart from prediction, AI-based optimisation of formulations enables the simultaneous analysis of a multitude of interacting parameters as well as the identification of formulation and process conditions associated with defined quality criteria. Inverse design is a further conceptual step away from the typical forward development of formulations to goal-oriented engineering. Inverse design has the power to considerably increase the available formulation design space by defining desired delivery features a priori and computationally searching for candidate formulations that can fulfil such objectives. Moreover, generative AI could facilitate the development of new delivery architectures, beyond the experimental combinations already examined. Computational uniqueness alone does not suffice for a pharmaceutical fit. Generated or predicted formulations need experimental validation, safety assessment, scalability assessment and clinical relevance validation. Key hurdles including limited and heterogeneous datasets, uneven experimental standards, model interpretability, external

validation, reproducibility, algorithmic uncertainty and increasing regulatory requirements continue to hinder the translational dependability of AI-enabled medication delivery. To address these restrictions, a multidisciplinary partnership between pharmaceutical scientists, computer researchers, formulation engineers, pharmacologists, clinicians and regulatory professionals is necessary. Overall, AI should be viewed not as a substitute for experimental pharmaceutical science, but as an additional layer of intelligence to expedite hypothesis generation, formulation optimisation and rational delivery-system building. The convergence of predictive modelling, intelligent optimisation, inverse design, generative algorithms and experimental validation will further accelerate, building a more systematic, inexpensive and adaptive framework for next generation drug delivery system development.

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13. AUTHOR CONTRIBUTIONS
Both authors contributed equally to the literature review, data collection, manuscript preparation, critical revision, and final approval of the manuscript.

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