AI-assisted Formulation Design for Improved Drug Delivery and Bioavailability

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Abstract:

The pharmaceutical sector is changing thanks to artificial intelligence (AI), which has improved drug discovery, development, and delivery. AI-assisted formulation design has been a viable strategy in recent years to enhance drug distribution and bioavailability. Machine learning algorithms are used in AI-assisted formulation design to optimise medication formulations. The most effective formulation for a given medicine is predicted by these algorithms after analysing enormous quantities of data on drug qualities including solubility, permeability, and stability. Drug bioavailability can be increased thanks to AI-assisted formulation design, which is one of its key benefits. Bioavailability refers to the amount of a drug that enters the bloodstream and reaches the intended target. Due to characteristics including poor solubility or quick metabolism, many drugs have low bioavailability. AI can boost medicinal efficacy and bioavailability by enhancing drug formulations. AI-assisted formulation design also has the potential to improve drug delivery. The process of getting drug to its intended target is referred to as drug delivery. Due to issues like poor solubility or stability, many medications have few delivery alternatives. AI can enhance drug delivery and enable new delivery strategies, such as targeted drug delivery, by optimising drug formulations. The design of formulations with AI assistance may help hasten the development of new medications. AI can quicken the formulation development process by lowering the number of tests required to determine the ideal formulation.

Keywords: Artificial intelligence, Bioavailability, Machine learning, Algorithms, Optimize, Permeability.

Introduction:

A branch of computer science called artificial intelligence is solely focused on building machines that can carry out tasks that might otherwise call for knowledge and input from humans.[1]. The rapidly growing field of artificial intelligence (AI) is transforming several industries, including the healthcare sector. In recent years, the field of drug delivery systems has seen encouraging results from the use of artificial intelligence (AI). John McCarthy coined the word "A.I." for the first time in 1956. AI can be used to create novel pharmaceuticals. The use of artificial intelligence in formulation development is essential. In the field of drug administration, a variety of artificial network types, including deep or neural networksare used. A key tactic to improve and offer a higher success rate for drug administration is to target the proteins used in drug distribution [2]. Artificial intelligence (AI) is the ability of a machine to mimic human cognitive functions.

Machine learning, which is a part of artificial intelligence (AI), is the process of applying algorithms and pattern recognition to find trends in data to support decision-making [3]. Machine learning, which depends on the capacity to identify patterns in the run or flow of inputs without using or supplying any form of instruction, is a key component of AI learning. Numerical regressions and categorization are included in this ability to learn while also assigning control. The category is established by classifying an object's membership in a category, using regression-compact, and collecting a number of numerical data. The ability to create appropriate and pleasing outputs from a given input is made possible by discovering new functions using output or input examples [4].Machine learning techniques can be used to analyse big datasets of drug activity in the body and predict drug reaction. This can be useful to develop drug delivery methods that are best for particular patient populations.

Artificial intelligence has been increasingly used by the pharmaceutical sectors over the last five years (fig. 1), revolutionising how researchers create new pharmaceuticals, cure ailments, and more.The algorithms are essential for developing the AI architecture for the process industry since they are a set of rules to adhere to when employing computing devices to compute or solve problems [5].

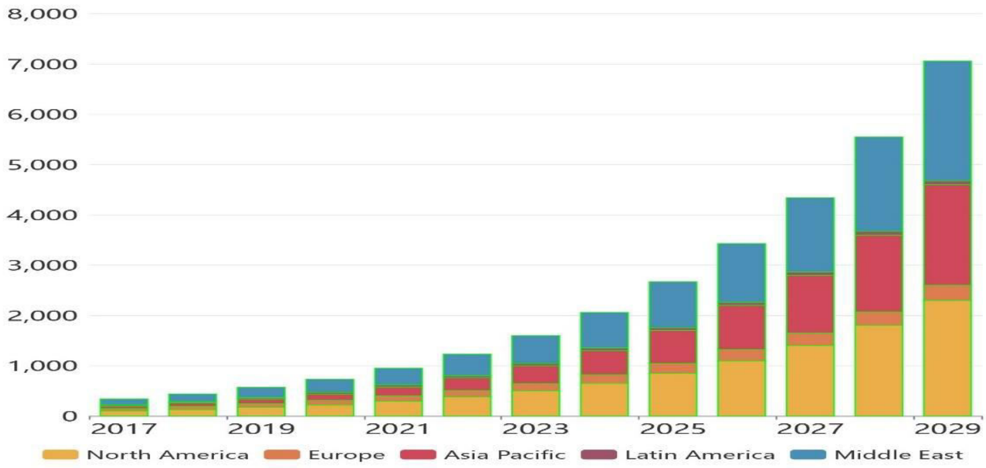

Fig. 1. Trends of rising AI usage in the pharmaceutical sector according to region

The medication is created in a form that is suitable to administer for intravenous usage or oral administration in the standard drug delivery method. Due to their increased requirement, decreased effectiveness, toxicity, and unfavourable side effects, these dose forms have been found to have strict limitations. To address the demands of the medical industry, new drug delivery technologies have been established or are being constructed to get around these restrictions [6] Traditional drug development methods, which often include high prices, demanding labour, and extensive lead times, typically involve a large amount of time between the identification of prospective drug candidates and the application of such novel therapies in the clinic[7].

The pharmaceutical sector has made extensive use of AI-based drug development, which is seen as a viable alternative to the current process. AI-based drug delivery systems have a number of benefits and the potential to completely transform the pharmaceutical industry by enhancing medication administration and reducing toxicity. Artificial intelligence has made it feasible to formulate more accurate and effective medicine delivery systems. Drug delivery is the process of giving a drug or pharmaceutical item to a patient in order to achieve the intended therapeutic outcome [8]. If AI is used to novel medication delivery systems, the field of medicine could see a revolution. AI-driven drug delivery systems can improve patient outcomes, reduce side effects, and promote therapeutic effectiveness.

AI-assisted formulation design has the potential to increase medication bioavailability, which is one of its key benefits. Bioavailability is the extent to which a drug becomes totally available to its designated biological destination(s). The more appropriate name for this phenomenon is bioavailability, which refers to the pace and proportion of an initial dose of a medicine that actually reaches the site of action or the physiological fluid realm from which the drug's intended targets have unfettered access. [9-11]. The pharmacokinetics paradigm incorporates the idea of bioavailability. Administration, bioavailability, clearance, and distribution are usually referred to as ABCD in the field of pharmacokinetics, which examines how medications move through the body. The dose and distribution of a medication are referred to as administration. Clearance is the process by which an active medication is removed from the bloodstream. When a drug is taken orally, distribution quantifies how far it can get to the body's fluid compartments; this definition assumes that distribution happens after absorption[12].

Artificial neural networks (ANNs), another name for layered-structure algorithms, are frequently used to model deep learning, a subfield of machine learning (fig. 3). Compared to traditional machine learning techniques, ANNs have better computational and predictive capabilities because they were designed to mimic the organic neuron structure found in human brains [13]. Artificial neural networks (ANN) and pharmacokinetic simulations are used to develop formulations for regulated release [14].Parallelism, imperfection, and failure are a few of the notable information processing characteristics that ANN possesses. Their capacity for discovery, tolerance, learning, non-linearity, resilience, and ability to drive ambiguous and imperfect information. Real-world complicated issues like optimisation, pattern classification, clustering, and pattern classification can be tackled with the help of ANNs. Applications for ANN models are numerous. The main kinds of ANN models are associating networks, features-extracting networks, and non-adaptive networks[15].

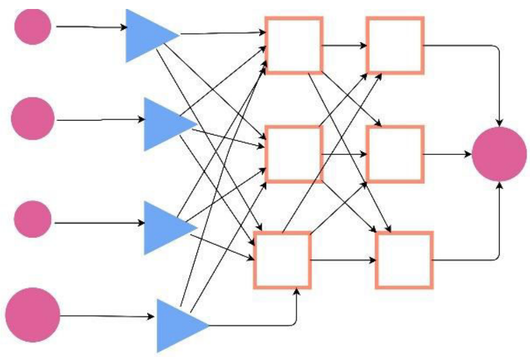

Fig. 2. ANN layered network

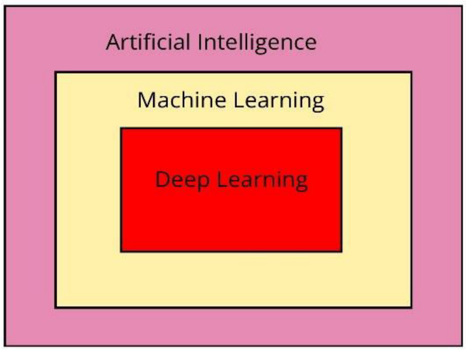

Fig. 3. Branches under AI

Robotics is anothercritical AI-related field. They require advanced surveillance and reporting carrying out activities such as item handling and navigation, as well as the related problems of mapping, localization, and motion planning.When it comes to size and the ability to provide precise medication, the robot has been shown to be significantly more effective than people. Manufacturing oral and injectable medications, especially hazardous chemotherapy drugs, is an example of robotics technological advancements abilities. With more space, the UCSF nurses and chemists could put their expertise to use by focusing on offering direct patient care and working with the doctors [16].

AI in drug formulation and delivery:

Many people in recent years have used AI-driven models successfully in the development of pharmacological dosage forms. Designing drug delivery systems that are best for particular patient populations can benefit from machine learning. Machine learning algorithms are one type of AI-assisted drug delivery system that is used to enhance drug compositions. Large datasets of drug behaviour in the body can be used to train machine learning algorithms to forecast the ideal formulation for a given drug [17].Recurrent neural networks and convolutional neural networks are two examples of Deep Learning algorithms that have been effectively used in the pharmaceutical sciences for a number of formulation-related activities, among these include identifying tablet flaws [18, 19], forecasting storage stability [20], forecasting particle flow ability [21], and forecasting medication dissolution profiles [22].

Tablet formulation using AI:

The optimisation of drug release, the forecast of tabletcollapse time, and the detected tablet flaws are just a few of the uses of AI in tablet formulations that will be covered in this part.

Optimizing drug release:

Galata et al. evaluated the use of three AI algorithms to forecast theHydrophilic matrix sustained-release tablet dissolving characteristics in a 2021 paper. In this study, data analysis and dissolution profile prediction were carried out using ANN, Ensemble of Regression Trees, and SVM.Likewise, results from Process Analytical Technology (PAT) and Critical Material Attributes (CMAs) were merged input information to build a database for modelling. Particle Size Distribution (PSD) was shown to be one of the most important factors for the model's prediction, according to the results. Additionally, according to the evaluation measures, ANN was shown to be the best accurate model among all models [23].

Prediction of disintegration time:

Deep neural networks were used to forecast the time at which pills would dissolve, according to research by Han et al. [24]. The enhanced maximum dissimilarity method (MD-FIS) was used in this work to divide the data from 145 medication formulations into groupings for testing and training. Data were gathered using literature mining. Dataset for testing and validation can be corresponding thanks to the notable sophisticated data selection method known as MD-FIS. For the modelling process, a deep neural network with ten hidden layers and 50 neurons in each layer was constructed. The improved deep neural network achieved good accuracies of 85% and 80%, respectively, in the validation and testing sets. [24].

Detection of tablet defects:

By combining XRCT and deep learning, researchers have successfully identified tablet flaws, expanding the scope of this technique's potential utilization[25]. Convolutional neural networks were investigated by Ma et al. for use in identifying inside tablet flaws. Various batches of tablets were produced for this investigation, and they were then captured by XRCT for additional analysis. The excipients in the tablets included mannitol and microcrystalline cellulose. A approach of picture augmentation was used, increasing the number of photos from 573 to 43,548. For the image analysis, a CNN with the three modules below was used: (A)UNet A, which removes pills from bottles; (B) Module 2, an automated analysis that locates certain pills; (C) UNet B, a statistical tool that can assess inner tablet construction flaws. The UNet neural network demonstrated up to 94% accuracy for seven batches of tablets during the model testing. The time, workload, and expense associated with product fault discovery may all be considerably reduced with the CNN approach. [18,25].

Capsules:

Drugs are contained in capsules, which have gelatin or other materials as the outer shell. Another popular solid dose form, particularly for oral delivery, is the capsule.There is, however, a dearth of literature addressing the use of AI techniques in the creation of capsule-based formulations. The drug powders have been encapsulated in a number of capsule forms, including soft gelatin, hard gelatin, modified release, and enteric capsules, to generate various drug release patterns. Zhou et al. showed that it is possible to find capsule faults by utilising an improved CNN. In this investigation, manually manufactured capsules with various faults such as perforations, concave heads, uncut bodies, oil stains, shrivelled, locked, or nested, were used. L2 regularisation and an Adam optimizer were features of the upgraded CNN that were employed to combat the model's overfitting. Support vector machines (SVM) and K-Nearest Neighbour (KNN) were also used in this study for comparison. When using this improved CNN model, the confusion matrix results demonstrated acorrectness of up to 97.56% for identifying capsule flaws [26].

Controlled release formulation design:

Pharmacokinetic simulations and trained ANN model and have been used to generate controlled release dosage forms. As inputs and outputs, respectively, formulation parameters and the cumulative proportion of the medication delivered at different time points were chosen [27].The pre-formulation stage of controlled release oral dose formulations may also include ANN models [28]. In order to examine the impact of formulation excipients on release characteristics and optimise medication formulations, sustained release formulations are made using fuzzy logic and ANNs [29–31]. In order to create controlled release formulations of clopidogrel, the effect of tablet components on drug release has been researched using the fuzzy logic algorithm and ANN analysis. By using ANNs and pharmacokinetics simulations to create complex drug formulations and controlled-release drug products, it was found that the experimental results and the predictions made by the ANN were in good agreement, indicating that the ANN was able to effectively model the relationships in the data. [32].

Solid Dispersion:

A rigid dispersion is one of the most crucial processes for dissolving dosage forms that are solid, and it frequently incorporates both drugs and polymeric. Both fusion-based methods, like warm-melt extrusion, and solvent-based methods, including coprecipitation and spray-drying, can be used to produce solid dispersions [33]. ANNs, mixed experimental design has been combined to create solid dispersions. The rate of drug dissolution was accelerated by solvent casting of solid carbamazepine-Soluplus®-poloxamer 188 dispersions using a three-layer feed forward MLP network and a mixed experimental design, the impact of solid dispersion composition on the rate of carbamazepine dissolution was evaluated. The ANN model and mixture experimental design did a decent job of characterising the link between the elements of solid dispersion and the proportion of drug released, even if the MLP network showed higher predictability than the latter[32,34].

Emulsion:

Stable emulsions have been made using ANNs that can simulate and optimise the intricate relationships between formulation parameters and their impact on product performance [35]. ANNs were employed in a study by Kumar et al. to create stable oil-in-water emulsions and to boost the amount of a fatty alcohol. The input data consisted of lauryl alcohol concentrations and time variables, while the outputs taken into consideration were zeta potential, viscosity, particle size and conductance. The validation trials revealed high accordance between experimental data and ANN-predicted values[36].

Transdermal Dosage form:

The vehicle composition for melatonin transdermal delivery has been optimised using ANNs and RSM [37]. The transdermal method, which likewise maintained steady-state plasma concentrations for the needed durations, prevented the exceptional first-pass metabolism of melatonin. A variety of solvents and solvent mixes were utilised to increase melatonin permeability and shorten lag time because the stratum corneum's strong hydrophobic nature prevents melatonin from reaching it. A numerous-layer feed-forward backpropagation network was created in order to identify the best solvent combinations for each answer and assess the inter-relativity between the replies. The experiment's outcomes were in line with what was predicted [32,37].Incorporating neural network technology, to find the chemical penetration enhancers for transdermal medication delivery, a screening technique has been created using GAs and theory-based quantitative structure-property relationship models [38].

AI assisted implants:

Coating the implants for topical delivery of anti-inflammatory or anti-infective medications has been recommended to treat the postoperative problems related to cochlear implantation [39]. The formulation factors and release of dexamethasone from the implant coatings were predicted using an ANN model. The ability of the ANN model to choose the appropriate formulation parameter levels was put to the test in order to give the optimal medicine release profile. The ANN model not only accelerated formulation design but also successfully anticipated the medication release profile from the implant device. The model's usefulness was established since the results were so closely related to the empirically observed values. [32,39].

AI assisted microchips for drug delivery:

The use of microchip drug delivery systems with the capability to autonomously alter drug concentration and release timing is a promising strategy for enhancing the safety, efficacy, and patient compliance for controlled and targeted therapeutic delivery [40]. For almost six months, a microchip implant containing electrical parts, power source and wireless communication technology have been in use [41] to administer controlled medication release followed by pulsatile release. The first clinical trial on patients with osteoporosis involved implantable microchips for medication delivery [42]. Controlled insulin administration and routine blood sugar monitoring can help to significantly reduce the risk of developing diabetic complications. It is advantageous in this case to integrate glucose monitors, control algorithms, mathematical models, and an insulin administration system. A single automated system for glucose monitoring and insulin delivery now combines thedose calculator, insulin pump, and glucose metre[43,44].

Formulation design by AI assisted 3D printing:

Numerous techniques, including pressure-assisted micro syringe, selective laser sintering, binder jetting, stereolithography and fused filament fabrication, have been used to create customised 3D-printed tablets [45]. To assure the quality of the products generated, factors such as printing speed, platform temperature, and nozzle temperature are continuously controlled during the manufacturing process. These factors may also have an impact on the drugs in vitro and in vivo release patterns [46]. In order to enhance 3D printing and lessen the workload involved with tests involving many factors, AI technologies have huge potential to be incorporated into this approach and identify the design.

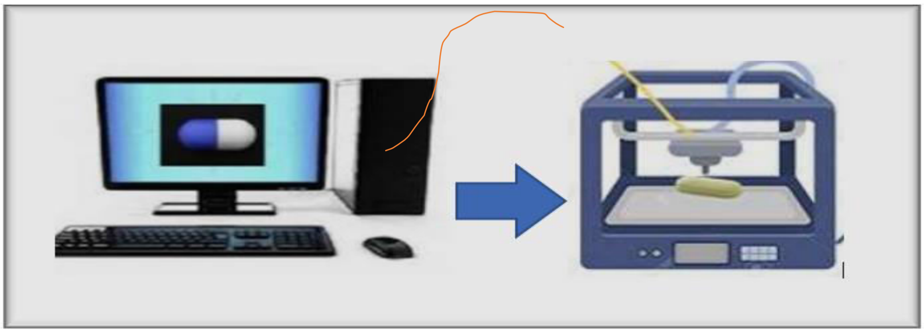

Fig. 4. 3D printing of tablet

The research has shown how artificial intelligence can be used to optimise processing settings during 3D printing. Using the ANN model, the effects of processing factors and the tablet surface area/volume ratio on the drug release from 3D-printed diazepam tablets were examined by Obeid et al. The infill density range of 20% to 100% and the infill pattern were employed as processing factors in this experiment with the dissolution rate as the target outcome. Initially, the interactions between various components were visualised and analysed using self-organizing maps (SOM). Following SOM analysis, surface area/volume ratio (SA/V) and infill density were chosen as input variables for additional modelling studies. Then a three-layer ANN with two neurons in the first layer, three hidden neurons in the second layer, and a fourth hidden neuron in the third layer. High dissolution rates were achieved with a zigzag infill pattern and a reduced infill density (50%) after ANN modelling and validation. Most crucially, the ANN model correctly predicted the rates at which diazepam pills would dissolve[25,47].

AI in nanotechnology for improved bioavailability:

For powerful drugs whose clinical development was unsuccessful because of their weak solubility, limited permeability, insufficient bioavailability, and other subpar biological properties, nanotechnology is a viable technique for the creation of drug delivery systems [48–50]. Using nanotechnology to make medications more bioavailable is a terrific idea. By combining it with

AI, nanotechnology's effectiveness can be further boosted.

In order to optimise medicine distribution, drug delivery nano systems have been designed, characterised, and manufactured using AI methodologies. The majority of AI approaches are employed for analysing and deciphering genetic and biological data. The medication development process has also been sped up by using this integrated strategy, which has also been successful in finding numerous small molecule activities and accurately predicting their behaviours[51].

The simulation is a key issue while operating at the nanoscale level. Since real optical images cannot be captured at the nanoscale, numerical models are typically used to interpret nanoscale images. But a variety of programmes are used to create these image representations, and often it might be difficult to include all the necessary parameters to create correct representations. In this aspect, AI efficiently creates simulations and easier-to-understand findings interpretations [52]. With the help of AI paradigms, it may be possible to get over nanotechnology's physical constraints and create nanoarchitectures with more powerful computers [53].

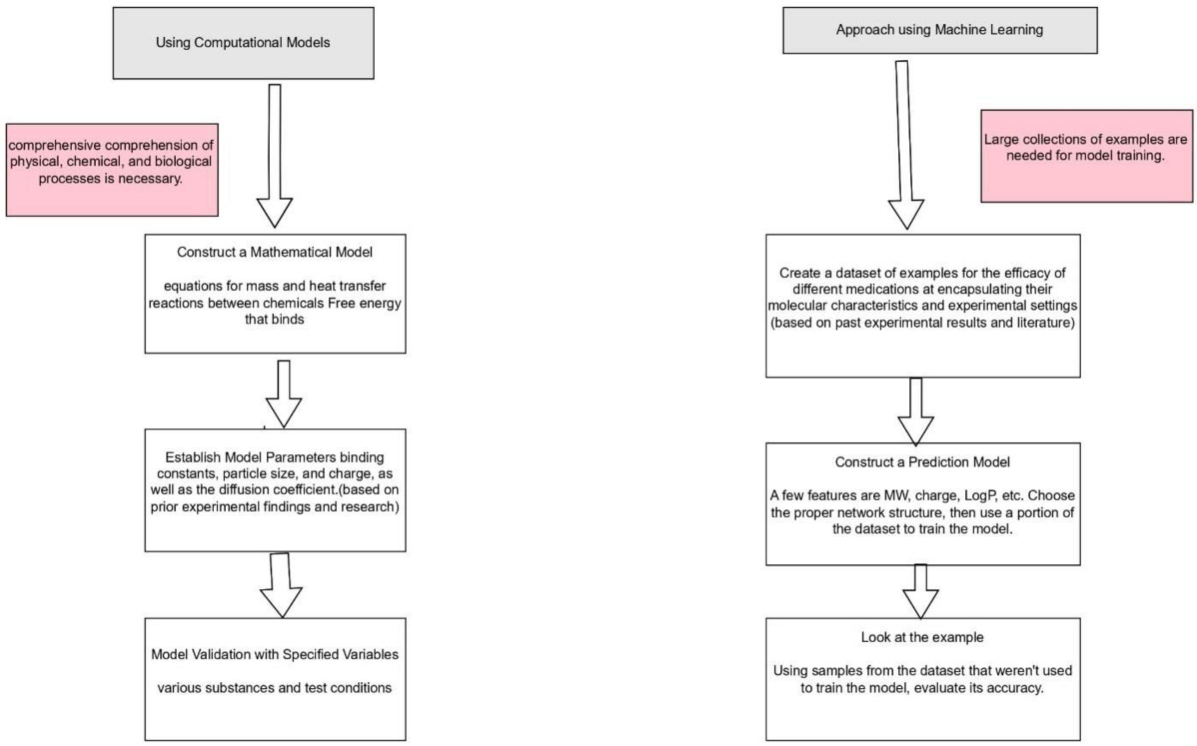

Fig. 5. AI in Nanoparticle Encapsulation

ANNs have been used in nanomedicine to simulate or analyse the synthesis of nanoparticles, significantly reducing the amount of work, time, and money required [54][55]. Amphiphilic nanoparticle phase behaviour has been simulated using QSPR modelling tools [56]. For determining the particle size and polydispersity index (PDI) of polymeric nanoparticles made using the emulsification solvent evaporation method, a mathematical model based on artificial neural networks (ANN) has been created [57]. Additionally, ANNs have been developed to predict the particle size and entrapment effectiveness of polyethylene glycol/polylactide (PEG/PLA) nanoparticles loaded with noscapine by taking into account a number of variables, such as the molecular weight of the polymer, the number of blocks, andpolymer to drug ratio. The polymer to drug ratio and the molecular weight of the polymer had, respectively, the most significant influence on particle size and entrapment efficacy. Using modelling and optimising techniques based on the spherical central composite design, the preparation of polymer-lipid hybrid nanoparticles for controlled administration of verapamil hydrochloride was optimised [58].

AI assisted robots for drug delivery:

A new technology that combines robotics and artificial intelligence to dispense drugs efficiently and precisely is called AI-assisted robots. These intelligent structures can process information, signal, sense, act, and communicate. They can also carry out cellular-level biological functions and distribute medications locally, improving the effectiveness and minimising the negative effects of conventional therapies[59–61]. The target identification rules, navigation rules, detection and attachment rules, collision avoidance rules, drug delivery rules, mission completion rules, and activation of the flush-out mode that results in bio nanorobot excretion are all included in the structure of bio nanorobot rules [60] [62,63]. DNA nanorobots have been activated by external nucleic acids that interact with their complementary counterparts on nanorobots to perform biosensing, initiate apoptosis, or carry medications [64–65]. Magnetic microrobots can be used to deliver drugs to the eye [66]. Wireless location and customization of medicine administration into the eye is a promising method for individualised treatment with little interference. Greater accuracy and precision in medicine administration are made possible by the application of AI in drug delivery robots. A patient's medical history, allergies, and other characteristics can be analysed by AI algorithms to find the optimum treatment plan and dose for each individual patient. The robots may also keep an eye on a patient's vitals and modify drug distribution as necessaryin order to quickly build medical capsule robots and intelligent medicine administration in a targeted manner, medication delivery capsules have been built employing a combination of several elements. an intelligent scheduler and a coil-magnet-piston device for controlled medication release. Experimental validation followed simulation of the magnetic force and the drug release curve [67].

Nu-bots:

Nu-bots, DNA-based nanobots, are powered by proteins, tiny molecules, or other DNA-based compounds. Nubots can be constructed from a several kinds of materials, including polymers, metals, and carbon-based materials, and typically range in size from 0.1 to 10 micrometres. They are equipped with various sensors and actuators that allow them to move through the bloodstream, identify target locations, and release drugs.The nu-bots contain a variety of biological circuit gates[64], [68-70].

Biohybrid:

A growing area of study called "bio-hybrid systems" mixes biological and synthetic components to develop new technologies with a variety of uses, such as biosensing, medication delivery and tissue engineering. One area of bio-hybrid systems research is in the development of Bio-nanoelectromechanical systems (Bio-NEMS).Bio-NEMS have the potential to revolutionize the field of drug delivery by providing targeted and controlled drug release. By using biological components, such as antibodies or peptides, Bio-NEMS can be programmed to recognize and target specific cells or tissues in the body. Once the Bio-NEMS reach their target, they can release their cargo of drugs or therapeutic molecules, providing a precise and effective treatment. [71,72].

Mechanism of action of nanobot:

Nanobots' ability to sense allows them to evaluate the different sensing jobs they are capable of. Determined through chemical and thermal sensors.How much nanobot actuation might be enhanced.At that distance, with an angular resolution corresponding to a 3 m diameter, nanobot's unique senses allow it to discern objects at a distance of about 4 m. Finding therapeutic targets and delivering medications are made possible by the behaviour of nanobots, which relies on random motions and chemical gradient detection. [73].

Nanobot assisted Drug Delivery for Cancer Diagnosis:

Nanobots, also known as nanorobots, are measured in nanometres, or one billionth of a metre. They have the power to fundamentally change a variety of medical specialisations, including how cancer is identified. Chemotaxis was discovered during the nanobot's in-vitro testing, and when the subject material was activated, the medication was delivered towards the target [74, 75]. An examination of the application reveals the use of magneto tactic bacteria. To safeguard magnetic iron oxide particles that magneto tactic bacteria spontaneously created, in-vitro liposomes with therapeutic payloads were utilised [76].

Challenges and Future Prospects:

Due to their higher costs and decreased efficacy, the pharmaceutical industry is currently having a difficult time developing new treatments. Improvements in AI algorithms, particularly in DL methods, as well as improved architectural technologies and simple access to massive data are signs of the third wave of AI. Numerous pharmaceutical businesses have partnered with AI corporations as a result of researchers' interest in using AI methods in medication development [77]. Researchers will be assisted by both current and future AI technology with such difficult tasks as integrating many forms of information, determining explanations for what is occurring, modelling, and eventually forecasting what will happen in a certain scenario. The medico-legal context46 in which AI technology will be applied comes first. Responsibility for medical mistakes is frequently not clearly defined, even under current medical rules. This position becomes considerably murkier when AI "bots" help or even autonomously deliver healthcare services more regularly[78].

In the realm of pharmaceutical research, neural networks can be used to a variety of application areas and produce models that are at least as good as those created using statistical techniques and more traditional modelling. As seen in this chapter, when independent factors are added to neural networks, genetic algorithms may forecast the collection of variables that will result in the best potential outcome. Voice recognition, image identification, and natural language processing are a few examples of artificial intelligence (AI) applications that have outperformed humans in terms of performances [79].

Artificial intelligence (AI) is being supported by governments all over the world in a range of industries and occupations. Other governments actively supported the use of AI in healthcare, while some actively supported private companies in creating useful AI applications. [80, 81] Another problem is that even after knowing how AI robots make therapeutic decisions, some people may still be sceptical. Due to the complexity of deep learning and other cutting-edge algorithms, the "black box" conundrum suggests that some decision-making processes might be murky. [82]. The creation of AI services must involve clinicians, and ideally, they should take the initiative in doing so. They must also evaluate the data that was used to develop the algorithms and exert strict control over its application.

By performing computations and difficult jobs, analysing data, and creating treatments with fewer adverse effects, the application of AI technologies can assist with a range of issues, including those related to nanotechnology. Successful AI-based methods produce biocompatible, reliable, and practical drug delivery systems that can overcome a variety of barriers and deliver precise dosage and targeted drug administration with the fewest possible safety concerns [83, 84]. With fewer experiments and lower costs, ANN-based approaches optimise drug release profiles and estimate drug pharmacodynamics and pharmacokinetic properties. Preferable to use intelligent systems with fuzzy logic for diagnostic reasons, better drug delivery efficiency, bio nanorobot navigation, and lower false-positive rates in cancer therapy. ANN models might not have a clear understanding of the mechanism underlying variable correlation. In order to create models that are more accurate, it also takes time, a lot of data, and a large sample size to produce a dependable ANN model. ANNs have the ability to model complex datasets and generate precise predictions of the clinical response to pharmaceuticals, however, it can be challenging to choose the right algorithms or datasets for ANNs-based drug development initiatives. [85].

Even after completing the appropriate regulatory processes, the introduction of AI-enabled apps would almost certainly face pushback. Clinical professionals have a history of adopting new technology slowly and preferring to stick with tried-and-true clinical care approaches. In order to prevent these applications from adding to clinicians' workload, it is crucial for developers and authorities to involve physicians in the design and testing of the applications[84,86].

AI is now utilised in drug discovery to find targets, find hits, improve leads, forecast ADMET, and design clinical trials. Despite tremendous advancement, a number of problems remain, including the two fundamental problems with high-quality data collecting. Lead optimisation is a problem in developing an effective medication with strong ADMET characteristics and target activities; nevertheless, these criteria are independent and sometimes in contradiction with one another. This issue can be resolved by carefully optimising each parameter and enhancing the model. Pharmaceutical companies struggle to recruit enough people for clinical research [87].

Conclusion:

In conclusion, AI-assisted formulation design offers a promising means of enhancing drug absorption and distribution. AI can improve therapeutic efficacy by optimising formulations and enabling innovative delivery methods. AI-assisted formulation design is projected to become a more crucial tool for the pharmaceutical business as the technology develops. Researchers can find the best formulations with enhanced drug delivery and bioavailability more quickly and effectively by using machine learning algorithms than by using conventional trial-and-error methods. This may result in the development of patient-specific, efficient medicines that eventually improve outcomes.Additionally, by finding novel drug candidates, determining efficacy, and creating formulations, AI-assisted formulation design helps quicken the drug development process. The combination of AI with nanotechnology, which includes nanobots, has proven to be a great strategy for improving bioavailability and drug delivery. This could lead to the development of more effective medication therapies that benefit patients and change the pharmaceutical business. While there are many advantages to AI-assisted formulation design, there are also difficulties that need to be resolved in order to guarantee the moral, responsible, and efficient application of AI in medication development.

Acknowledgement:

The authors would like to express their gratitude to the Director Dr. (Col.) A. Garg, Joint Director Dr. Manoj Goel, KIET's Group of Institutions, Ghaziabad, and Principal Dr. K. Nagarajan of the KIET School of Pharmacy for their inspiration and overall support.

Conflict of Interest:

Authors declare no conflict of interest.

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