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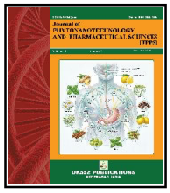

Review Article : Open Access

AI-driven novel approaches in 3D and 4D-printing for drug delivery systems

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Abstract

The unification of artificial intelligence (AI) and 4D printing heralds a new wave of advancement in the creation of smart, site-specific, and controllable drug delivery systems, with the impacts of a transformative assembly through novobiocin on coli Rab7 found in a study. Consequently, combining adaptable printing with AI-enabled predictive modelling enables the development of dynamic dosage forms responsive to situational cues, such as changes in light, pH, or high-enzyme-expressing locations. Due to advances in additive manufacturing science, both the efficiency and predictive accuracy of designing solid dosage forms in the pharmaceutical industry are improved through processes that automatically optimise, control performance, and process control through AI modelling and simulation. Wherein consequential roles of 4D materials pertain to fabricated architectures that undergo precise functional or morphological modification in response to external stimuli, all of which effecting tailor made and responsive drug delivery for all purposes. With hydrogels, magnetic insulated materials, as well as shape-memory systems, if the temporal dimension could be added to additive manufacturing, it would make the 3D printing constructs undergo regulated in situ transformations in their form or shape owing to external stimuli; this will work perfectly for both on-demand and point-targeted release of drugs for different therapeutic regimens and varied functionality. In addition, with AI-driven algorithms, we can rapidly simulate and optimise release kinetics as well as mechanical behaviour, resulting in greatly reduced experimental trial-and-error cycles. However, while there are now issues like material standardisation, scalability and regulatory approvals, evolution in Smart material design along with machine learning frameworks is making way for adaptive pharmacotherapy and personalised drug delivery.

1. Introduction

4D printing is a modified version of the existing conventional 3D printing by the addition of the time dimension. This allows for structural and functional changes and responses of the printed structures upon external stimuli, such as temperature, pH, moisture, or magnetic field. These dynamic abilities give great benefits in particular within the field of pharmaceutics, where responsive drug delivery systems and personalised medical devices can be created (Abdullah and Okay, 2023). In 2013, the concept of 4D printing was introduced by researchers at the Massachusetts Institute of Technology, who demonstrated that 3D-printed structures have the ability to perform programmed transformations in response to specific environmental conditions. Since then, rapid development has been observed in this field concerning material sciences, printing technologies, and computational modelling. Within the pharmaceutical area, 4D printing became a very promising approach in solving challenges such as drug release control, patient-specific dosing, and the development of intelligent medical devices (Antezana *et al*., 2023). Recent studies were dedicated to the detailed explanation of new materials and techniques that offer further improvement of performance in 4D-printed pharmaceutical systems. For example, the incorporation of magnetic-responsive bilayer hydrogels opens an opportunity for remote control of drug release and is promising for new horizons in targeted drug therapy (Kurien *et al*., 2025). With artificial intelligence integration with 4D printing in the optimisation of the drug design process and enhancement of functionality in pharmaceutical devices, the prospects are high. This can contribute to improving the prediction of material behaviour, optimisation of printing parameters, and personalisation of drug delivery systems through data from individual patients (Gazzaniga *et al*., 2023).

2. Pharmaceutical advantages and therapeutic relevance

2.1 Personalised drug delivery

The use of responsive materials in 4D printing enables the development of personalised dosage forms tailored to individual patient therapeutic requirements, thereby enhancing treatment efficacy while minimising adverse effects. These systems are designed with stimuli-responsive materials that can exert site-specific or time-controlled release of drugs upon certain stimuli, hence enhancing patient compliance and improving therapeutic outcomes (Appuhamillage *et al*., 2024).

2.2 Responsive materials

Materials used for 4D printing can respond to a specific physiological trigger that allows on-demand release of therapeutic agents. Such materials, when subjected to changes in temperature or pH, can swell or shrink, like hydrogels, to allow controlled drug release in the gastrointestinal tract (Bernatoniene *et al.,* 2025).

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2.3 Complex geometries

It allows the fabrication of complex structures that can perform multiple functions, such as drug release and mechanical support, within one device. This capability is useful in developing either implants or scaffolds for tissue engineering applications (Aguilar and Herrada-Manchón, 2023).

2.4 Reduced manufacturing complexity

The 4D printing technique will continue to simplify the conventional fabrication of complicated pharmaceutical devices through cost and time reduction. This technique, in turn, allows for the fabrication of multi-functional devices in one step, hence reducing several manufacturing steps and materials (Gazzaniga *et al*., 2023).

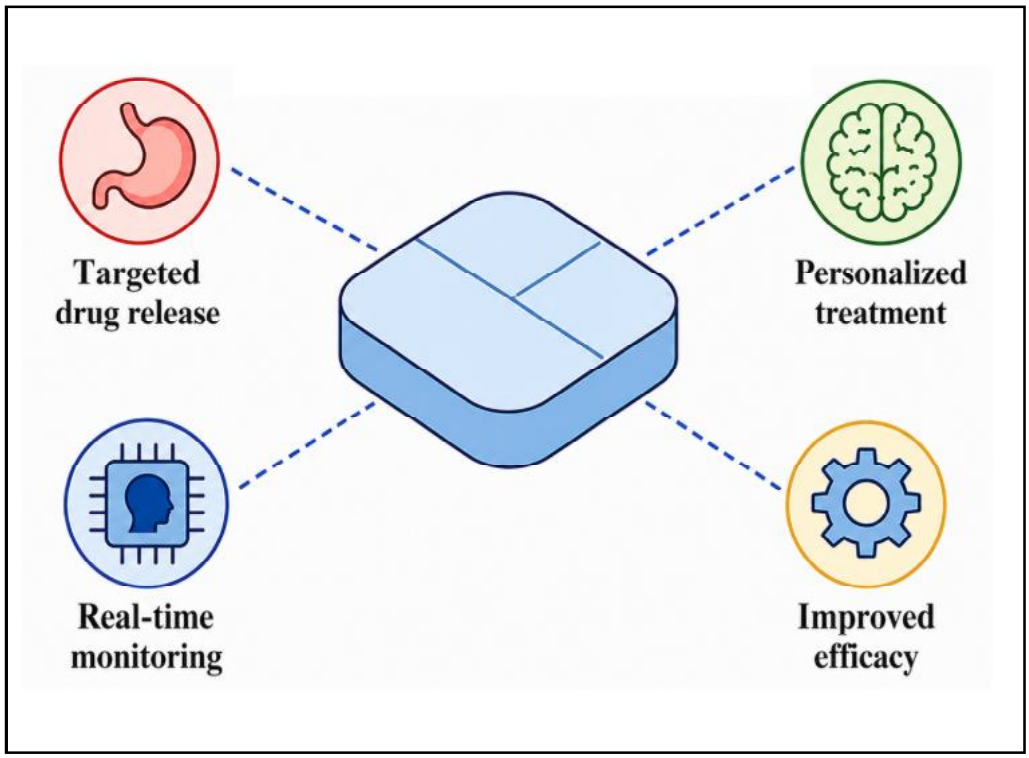

Figure 1: AI-integrated 4D printing in drug delivery.

3. Technical and regulatory constraints

3.1 Material limitations

The process for the development of biocompatible and biodegradable materials with controlled transformations is just at its initial stages. Even though many polymers have been tried, a material with desired properties for pharmaceutical applications is yet to be achieved (Sautha *et al.,* 2025).

3.2 Regulatory hurdles

Regulatory approval for 4D-printed pharmaceuticals involves a complex process that includes elaborate testing on safety and efficacy. Regulatory agencies are supposed to set guidelines for the performance and quality testing of these new systems (Aguilar and Herrada-Manchón, 2023).

3.3 Manufacturing scalability

Translation of these 4D printing processes from the laboratory scale to the industrial scale remains one of the greatest challenges. Issues related to reproducibility, quality control, and cost-effectiveness have to be overcome before widespread use is possible.

3.4 Cost considerations

The initial investment in 4D printing technology and materials can be high, acting as a barrier to wide-scale adoption. Yet, costs are expected to fall once the technology matures to become more accessible, thus being made feasible for pharmaceutical applications (Gazzaniga *et al.,* 2023).

4. Types of 4D printing in pharmaceutics

4D printing systems in pharmaceutics are classified according to their mechanism of responsiveness, material composition, and design complexity.

4.1 Shape-memory systems

These systems are some of the earliest and most widely studied constructs in 4D printing of pharmaceuticals. These are based on polymers that, under the action of environmental stimuli-such as temperature, pH, or specific solvents-can assume a pre-programmed shape. Thermo-sensitive polymers have been specifically developed, showing improved site-specific delivery and therapeutic efficacy due to specific release in targeted areas of the gastrointestinal tract (Elbadawi *et al*., 2024; Li *et al.,* 2025).

4.2 Hydrogel-based systems

These systems dominate 4D pharmaceutical research because of their unique swelling/shrinking ability, and they can be readily tuned. Single- or dual-responsive hydrogels can precisely provide spatiotemporal control for drug release. Advanced designs include magnetic-responsive or light-sensitive hydrogels that could remotely control drug delivery and bring significant benefits to personalised therapies (Elbadawi *et al.,* 2024; Appuhamillage *et al.*, 2024).

4.3 Layered or bilayer structures

These systems have advantages in realising high functionality in the 4D-printed device by combining more than one material with different responses. Stimuli-responsive bilayers or multi-material composites enable controlled bending, folding, or swelling, especially for implants and tissue scaffolds. Biocompatibility and biodegradability of these layers remain crucial for translation into clinical applications (Imam *et al*., 2021; Kurien *et al*., 2025; Salama, 2025). AI-powered smart systems are also being regarded as the next developing stage in 4D pharmaceutics in predicting the behaviour of stimuli-responsive materials. Artificial intelligence helps a lot by reducing high losses in health and optimisation required in printing parameters and finally in the personalisation of drug release profiles relative to patient-specific data. These complex drug delivery platforms permit combinations of multi-drug formulations and personalised medicine, offering maximum therapeutic efficacy with all the safety.

In general, 4D printing systems of different hybrid architectures involve AI-assisted design optimisation along with shape-memory material responsiveness and hydrogel responsiveness such that radiative precision of an optimised beam stimulates material aid transformation, helping in realising highly controllable spatiotemporal material behaviour including programmable transformations to applied pulse of environmental temperature, pH or moisture. Certain 4D printing systems(commands) offer remarkable mechanical stability, tunable kinetic parameters of drug release, and enhanced adaptability to custom requirements with medicament. Hence, they represent a significant step in the development of the next generation of intelligent and responsive patient-specific pharmaceutical delivery devices (Gazzaniga *et al.,* 2023; Segneanu *et al.,* 2025). Thus, they represent an important development toward the fabrication of next-generation, patient-specific pharmaceutical delivery devices with intelligent and responsive capabilities.

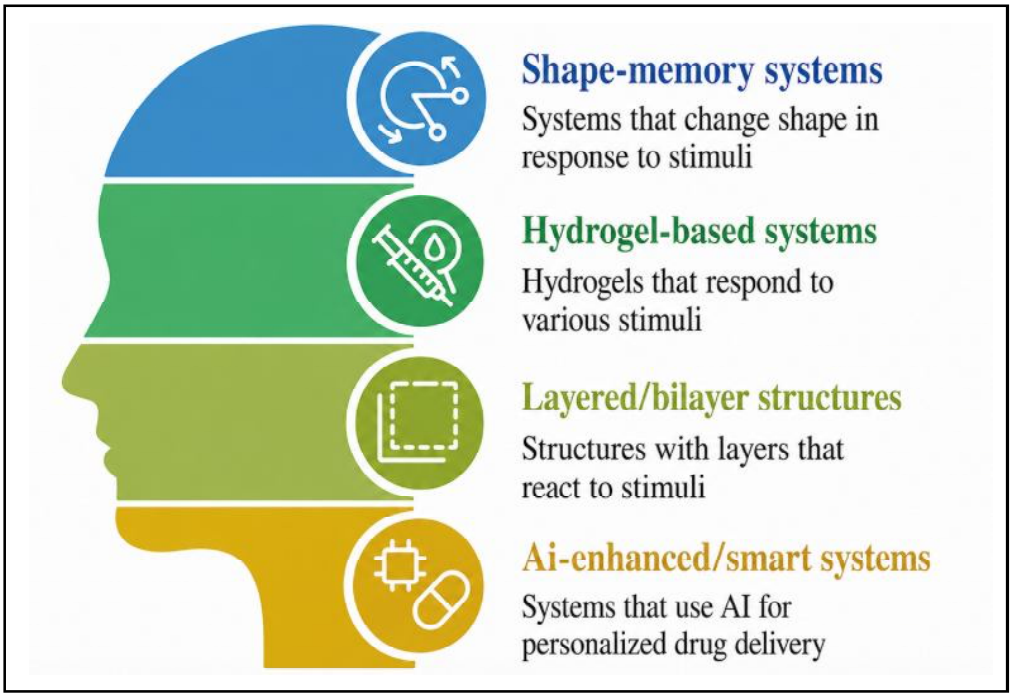

Figure 2: Types of 4D printing in pharmaceutics.

5. Applications of AI-integrated 4D printing in pharmaceutics

4D printing of pharmaceuticals indeed ushers in a new frontier in drug delivery owing to the possibility of realising dynamic, stimulus-responsive dosage formats which may aim at specific diseases, organ systems, or tissues with enhanced therapeutic efficacy and reduced systemic side effects.

5.1 Gastrointestinal disorders

Thermo- and pH-responsive hydrogels can release drugs at specific regions of the gastrointestinal tract, such as the stomach or intestine. This ensures protection against gastric degradation and liberation at a site where absorption is maximum (Abdullah and Okay, 2023; Appuhamillage *et al.,* 2024).

5.2 Cardiovascular diseases

4D-printed implants or stents with shape-memory properties can adapt to vascular geometry, thus enabling local drug elution for cardiovascular interventions, such as anti-proliferative drugs against restenosis (Li *et al.,* 2025).

5.3 Oncology

Stimuli-responsive hydrogels and multi-layered structures allow site-specific delivery of chemotherapeutic agents, reducing systemic toxicity. Magnetic-responsive hydrogels can further enable the remote control of drug release, so important in solid tumour targeting (Kurien *et al.*, 2025; Li *et al.*, 2025).

5.4 Intravesical and urological applications

Custom 4D-printed intravesical devices can release drugs in a controlled, patient-specific manner within the bladder. The result of this is improved adherence to and better therapeutic outcomes in urinary tract disorders.

5.5 Neurological and localised therapy

4D systems based on bilayer or hydrogel systems may provide sustained delivery of neuroprotective agents or analgesics to targeted regions in the brain or nerves, therefore improving therapeutic windows by reducing off-target effects.

5.6 Personalised medicine

AI-enhanced 4D printing allows the customisation of drug doses, release kinetics, and device geometry based on patient-specific data, revolutionising precision medicine in chronic diseases and polypharmacy management (Segneanu *et al.*, 2025; Sharma and Jain, 2023).

5.7 Administration routes

The dosage forms developed through 4D printing might be suitable for oral, buccal, transdermal, intravesical, implantable, and injectable routes depending on the material and design. This can achieve spatiotemporal control of drug release and overcome the limitations of traditional dosage forms (Meshram *et al.,* 2024*;* Elbadawi *et al.*, 2024).

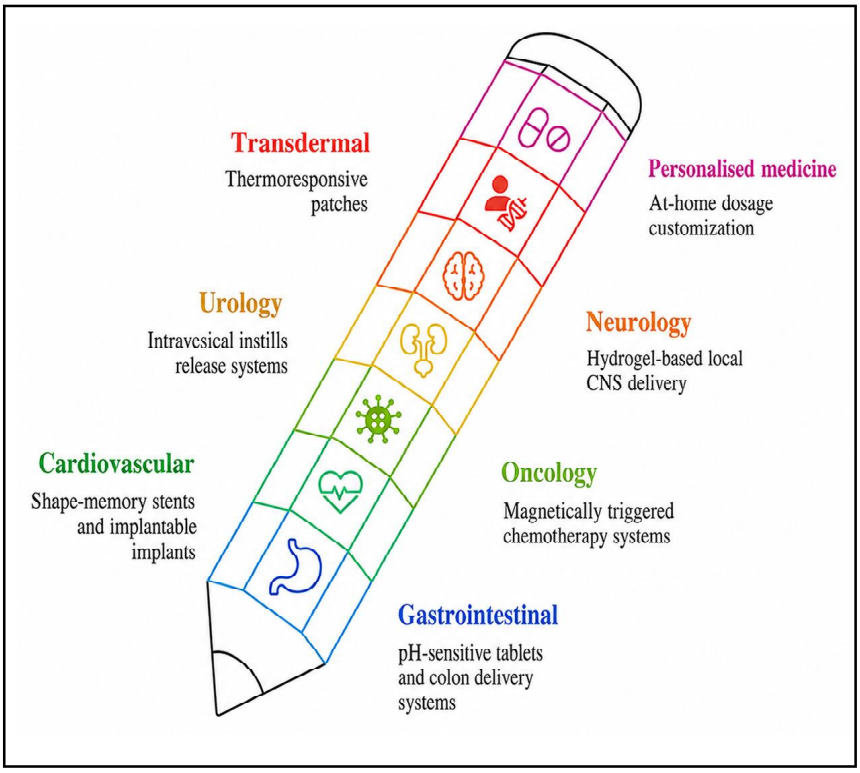

Figure 3: Applications of AI-integrated 4D printing in pharmaceutics.

6. Ideal characteristics of 4D-printed pharmaceutical systems

4D-printed drug delivery systems should ideally possess the following characteristics for effectiveness

6.1 Biodegradable and biocompatibility

The materials should be biocompatible inside the human body and able to degrade without residues that could be harmful (Sautha *et al.*, 2025). Predictable and tunable responses: The system must be able to provide predictable and controllable transformations in response to a given stimulus (Bernatoniene *et al.*, 2025).

6.2 Mechanical integrity

The structures printed must maintain their functionality and stability under physiological conditions (Aguilar and Herrada-Manchón, 2023).

6.3 Scalability and reproducibility

The processes should be adaptable to large-scale manufacturing while ensuring the uniformity of batches (Gazzaniga *et al.,* 2023).

7. Drug selection criteria for 4D-printed dosage forms

The selection of the ideal drug candidate for 4D-printed dosage forms depends on several factors

7.1 Physicochemical properties

Drugs shall present stability in conditions of printing, such as temperature, shear stress, and light exposure, without degradation. Solubility and permeability characteristics are very important to ensure predictability of release from hydrogels or layered structures (Abdullah and Okay, 2023; Appuhamillage *et al.*, 2024).

7.2 Therapeutic window

The main beneficiaries of 4D printing are drugs with narrow therapeutic indices, whereby the release kinetics can be precisely controlled to avoid under- or overdosing (Gazzaniga *et al.,* 2023; Segneanu *et al.,* 2025).

7.3 Targeted action requirement

Drugs that demand site-specific delivery, such as chemotherapeutics, antibiotics, or neuroprotective agents, are ideal candidates, since 4D systems enable spatially controlled drug release.

7.4 Molecular size and biocompatibility

Small to moderate molecular weight drugs are preferred for diffusion-controlled release from hydrogel or bilayer systems. Drugs must also be compatible with excipients and biopolymers used in printing (Appuhamillage *et al*., 2024; Salama, 2025).

7.5 Stability of physiological conditions

Drugs should be stable at different pH, temperature, or enzymatic conditions, especially for oral or implantable dosage forms. Drugs sensitive to gastric acid can be protected by means of pH-responsive layers (Abdullah and Okay, 2023; Li *et al*., 2025).

7.6 Combination therapy feasibility

Drugs that can be co-formulated for multi-drug release are preferred, availing the multi-layered or compartmentalised design of 4D-printed systems (Meshram *et al*., 2024*;* Sharma and Jain, 2023).

7.7 Patient compliance-related considerations

The drugs that require less frequent dosing or a controlled release are highly suitable for 4D systems in improving adherence. AI-assisted customisation can further enable patient-specific dosing

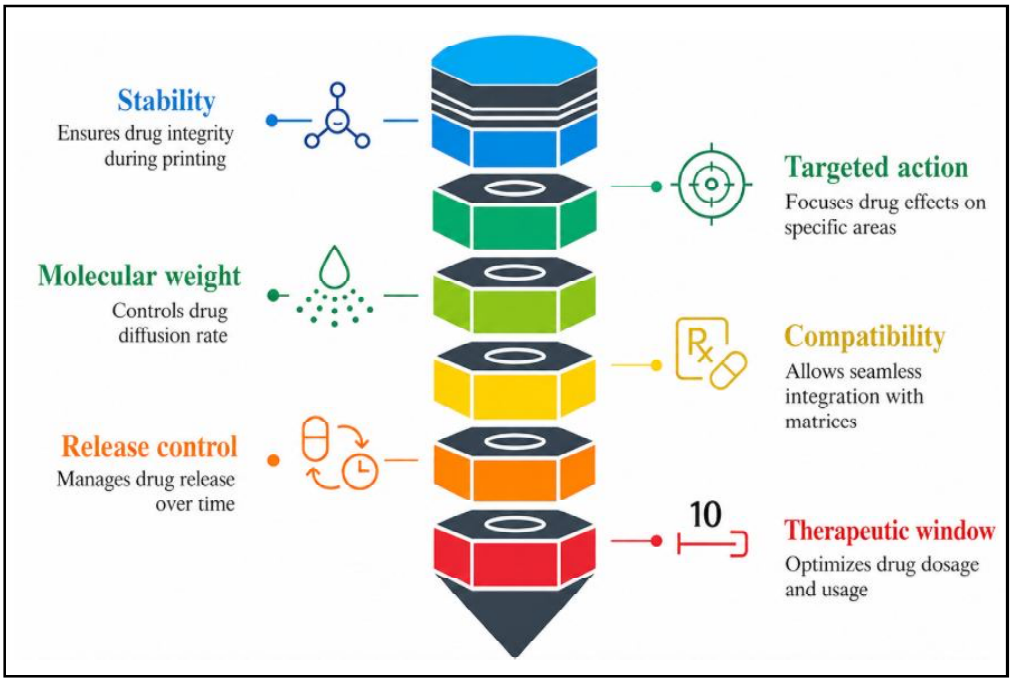

Figure 4: Key attributes in drug selection criteria. (Sharma and Jain, 2023; Segneanu *et al*., 2025).

8. Composition/excipients of 4D-printed dosage forms

The composition of the 4D-printed pharmaceutical system is critical in ensuring stimuli-responsiveness, mechanical stability, biocompatibility, and controlled drug release. Excipients should be selected according to the desired response, route of administration, and printing technology.

8.1 Polymers (Hydrogels and shape-memory polymers)

In their structure, hydrogels are based on poly (vinyl alcohol), polyethylene glycol, and natural polysaccharides. They show the ability to swell-deswell and change shape depending on temperature, pH, or magnetic stimuli (Salama, 2025). Shape-memory polymer materials (most often polyurethane derivatives) allow reversible structural changes, which is critical for implantable devices or stents (Bernatoniene *et al.,* 2025).

8.2 Plasticizers

Plasticizers, like glycerol or triethyl citrate, enhance the flexibility and consequently the processability during printing. They allow printed constructs to maintain their mechanical integrity while making shape transformations smooth, according to references (Appuhamillage *et al*., 2024; Elbadawi *et al.*, 2024).

8.3 Crosslinking agents

Glutaraldehyde or other chemical or physical crosslinkers, calcium ions, and photochemical UV-induced crosslinking agents were used to stabilise hydrogel networks and control drug diffusion rates (Salama, 2025).

8.4 Stimuli-responsive additives

Additional functionality can be built by incorporating magnetic nanoparticles, photothermal agents, or pH-sensitive moieties that enable remote control or environment-specific activation.

8.5 Binders and viscosity modifiers

The rheological properties of bio-inks are controlled by agents such as hydroxypropyl methylcellulose or sodium alginate, making deposition behaviour predictable during printing (Appuhamillage *et al*., 2024; Li *et al*., 2025).

8.6 Drug loading agents/carriers

Poorly soluble drugs can be made more soluble by the complexation of cyclodextrins or delivery by lipid nanoparticles, which can provide more stability and better controlled release. This is especially true for hydrophobic drugs or sensitive molecules.

8.7 Biocompatibility enhancers/degradation modulators

Natural polymers such as gelatin, chitosan, or hyaluronic acid are added to enhance biocompatibility and control degradation in physiological environments. A careful combination of the excipients used will ensure that the 4D-printed dosage form is mechanically stable, responsive to stimuli, biocompatible, and capable of controlled site-specific drug release-the cornerstone of its therapeutic advantage.

9. Manufacturing of 4D-printed dosage forms

The manufacturing of 4D-printed dosage forms integrates advanced printing technologies, materials science, and pharmaceutical principles to accomplish precise, patient-specific drug delivery systems. The general steps involved in the process are usually as follows:

9.1 Design and modelling

It involves the design of a 3D CAD model of the dosage form with integral structural features, drug-loading compartments, and stimuli-responsive regions. Computational tools coupled with AI algorithms are capable of optimizing the design for drug release kinetics and mechanical behaviour.

9.2 Bioink preparation

Polymers, excipients, and drugs are blended into a printable bioink. Viscosity modifiers and plasticizers are added to adjust rheological properties for smooth extrusion and shape fidelity (Appuhamillage *et al*., 2024; Li *et al*., 2025; Elbadawi *et al.,* 2024).

9.3 Printing process

Various 3D printing techniques have been adapted for 4D printing, including extrusion-based printing, stereolithography, and inkjet bioprinting. The layer-by-layer deposition allows complex geometries and multi-material constructs (Abdullah and Okay, 2023; Bernatoniene *et al.,* 2025; Salama, 2025).

9.4 Crosslinking/post-processing

After printing, the constructs are crosslinked physically (temperature, ionic) or chemically (UV, glutaraldehyde) to stabilise their structure and define drug-release profiles (Appuhamillage *et al*., 2024; Salama, 2025).

9.5 Drug loading

With some systems, drugs can be loaded after printing by soaking, diffusion, or infusion into hydrogel matrices to maintain drug stability (Sharma and Jain,2023; Li *et al.,*2025).

9.6 Drying and sterilisation

The final dosage forms may undergo freeze-drying, supercritical drying, or mild sterilisation techniques that are compatible with sensitive drugs and polymers (Appuhamillage *et al*., 2024; Elbadawi *et al.,* 2024).

9.7 Quality control

Evaluation of mechanical strength, shape-memory performance, stimuli responsiveness, and *in vitro* drug release kinetics will help to ensure that the dosage form meets pharmaceutical standards. AI-based predictive models can be used to anticipate performance across patient populations (Gazzaniga *et al*., 2023; Agarwal *et al*., 2023).

9.8 Packaging and administration

Herein, custom 4D-printed dosage forms can be packaged for oral, implantable, or transdermal administration depending on the design and target site (Imam *et al.,* 2021; Kurien *et al*., 2025). This integrated approach enables the fabrication of customised, responsive, and complex pharmaceutical devices through 4D printing, which is otherwise difficult to achieve by conventional manufacturing methods.

10. Conclusion and future perspective

4D printing in pharmaceutics is an art of drug delivery technology that combines the structural precision of 3D printing with stimuli-responsive or "smart" materials to manufacture progressive approaches, patient-specific dosage forms. However, these systems can perform controlled transformations in response to different external or physiological cues such as temperature, moisture, magnetic field, or enzymatic activity and offer site-specific and temporally regulated drug release, consequently resulting in enhanced therapeutic efficacy with minimal systemic adverse effects and better patient compliance across a wide range of therapeutic domains, which may include GI, Cardiac, CNS and oncology among others. The integration of shape memory polymer, hydrogels, and multilayered architectures along with AI-based optimisation can further enable the creation of personalised, multi-drug and on-demand drug delivery systems for enabling spatiotemporal control over the drug release kinetics and custom-designed formulation depending on individual requirements, which is unattainable with conventional dosage forms. Despite such unique benefits, challenges persist in terms of manufacturing scalability, regulatory validation, biocompatibility, and the long-term stability of 4D printed constructs. Ongoing progress in the field of materials science, computational modelling, and AI-driven predictive analytics will help overcome these obstacles, thus expediting clinical translation further, thereby positioning it to be accessible and adaptable in the real environment. Four-dimensional printing marks

a milestone within the pharmaceutics domain where development of smart, adaptive, patient-specific therapeutic delivery mechanisms will change the view of personalised medicine and precision drug delivery forever.

Availability of data and material

All data are provided within the manuscript.

Authorship contribution statement

Safura Ayesha Mujeeb: Contributed to conceptualisation, supervision, methodology, validation, manuscript reviewing and editing, and overall guidance throughout the study. **Chundi Soumya:** Contributed to data curation, investigation, formal analysis, software handling, visualisation, and manuscript writing.

Consent for publication

All authors gave their full consent for publication and submission to this journal.

Conflict of interest

The authors declare no conflicts of interest relevant to this article.

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Ethics approval

Not applicable.

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