



# **Prediction of Mechanical Properties of 3D Printed Particle-Reinforced Resin Composites**

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Abstract: This review explores fundamental analytical modelling approaches using conventional composite theory and artificial intelligence (AI) to predict mechanical properties of 3D printed particlereinforced resin composites via digital light processing (DLP). Their mechanisms, advancement, limitations, validity, drawbacks and feasibility are critically investigated. It has been found that conventional Halpin-Tsai model with a percolation threshold enables the capture of nonlinear effect of particle reinforcement to effectively predict mechanical properties of DLP-based resin composites reinforced with various particles. The paper further explores how AI techniques, such as machine learning and Bayesian neural networks (BNNs), enhance prediction accuracy by extracting patterns from extensive datasets and providing probabilistic predictions with confidence intervals. This review aims to advance a better understanding of material behaviour in additive manufacturing (AM). It demonstrates exciting potential for performance enhancement of 3D printed particle-reinforced resin composites, employing the optimisation of both material selection and processing parameters. It also demonstrates the benefit of combining empirical models with AI-driven analytics to optimise material selection and processing parameters, thereby advancing material behaviour understanding and performance enhancement in AM applications.



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**Copyright:** © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). **Keywords:** digital light processing (DLP); additive manufacturing (AM); particle-reinforced resin composites; mechanical properties; material optimisation; empirical modelling; artificial intelligence (AI)

# 1. Introduction

Vat polymerisation (VP) encompasses several AM techniques, including stereolithography (SLA), digital light processing (DLP) and masked stereolithography (MSLA). These methods use UV light to selectively cure liquid resins, creating precise 3D models layer by layer [1,2]. While sharing the fundamental principle of light-induced polymerisation, each technique offers unique advantages in terms of precision, speed and material compatibility [3]. Such methods produce desired parts with excellent mechanical properties, highquality surface finish and high-resolution features [4,5]. VP offers numerous advantages, including high-precision fabrication, rapid printing speed, as well as the capability to work with a variety of materials, such as nanocomposites and biobased photopolymers [6–9].

SLA utilises a laser to cure the resin dot by dot, ensuring precise control over the curing process and resulting in high-resolution prints with fine details [10,11]. On the other hand, DLP projects the light through an entire layer using a digital micromirror device (DMD) or a projector for faster printing speed and simplified operation when compared with SLA [12,13]. MSLA printers, also known as daylight polymer printing (DPP), depend on a screen to polymerise the resin layer by layer, resulting in cost-effective 3D printing solutions [14]. Mechanical properties of parts produced by these VP techniques

can vary significantly based on specific methods used and processing parameters [13]. Understanding these variations is crucial for accurately predicting and optimising mechanical properties of 3D printed particle-reinforced resin composites. Figure 1 illustrates key features, differences, and comparative precision values, build volumes and print rates of such 3D printing techniques.



		once
Decent precision	High precision	Mediocre precision
Scalable build volume	Limited build volume	Mediocre build volume
Low print rate	Fast print rate	Mediocre print rate

Figure 1. Comparison of different 3D printing techniques, including SLA, DLP and MSLA, with their common features and differences [15].

Mechanical properties of parts produced by VP techniques can vary significantly based on several parameters, including print orientation, post-curing process, printing parameters (e.g., layer thickness, infill density, etc.) and material formulation. These variations are particularly essential when predicting the mechanical properties of particle-reinforced resin composites [11,16–18]. Pop et al. [17,18] reported that such printing parameters affected both the tensile and flexural properties of resulting parts using SLA and DLP. On the other hand, material formulation is also quite vital, as evidenced by Wada et al. [19] with higher flexural strength, flexural modulus and fracture toughness in DLP-printed specimens, as well as superior Vickers hardness and smoother surfaces for MSLA-printed counterparts. In addition, special resins used for specific dental and surgical applications make a positive contribution to mechanical properties, as evidenced by Park et al. [20] and Lai et al. [21].

The selection of 3D printing techniques like SLA, DLP or MSLA depends primarily on specific application requirements, with each technique offering unique merits with respect to print speed, print resolution and mechanical properties. For instance, SLA is prone to producing parts with exceptionally smooth surfaces and intricate details, particularly used for small-scale and high-detail applications [15]. Semary et al. [22] reported that SLA offers far higher accuracy than DLP when used to print surgical guides for dental implants. Lee et al. [15] reported the highest flexural strength of  $150.8 \pm 7.93$  MPa could be achieved in 3D printing denture models using SLA, which was followed by  $133.39 \pm 12.66$  MPa with DLP and  $133.28 \pm 9.39$  MPa with LCD. Park et al. [23] indicated that decreasing layer thickness in SLA increased the glass transition temperature ( $T_g$ ) due to the effect of print orientation. DLP printers are revealed to print specimens with significantly high flexural strength, flexural modulus and fracture toughness when compared with SL and MSLA printers [19]. It is evident that mechanical performance of 3D printed parts can be impacted by various printing techniques. DLP can be characterised by good surface quality

despite pixelated appearance on curved surfaces arising from voxel-based structures [24]. Notwithstanding such minor drawbacks, DLP yields higher mechanical strength and stress resistance than SLA, which is more feasible for functional prototypes and applications with good durability [19].

MSLA is a hybrid technique between SLA and DLP, which relies on the use of MSLA screens to mask UV light in order to selectively cure entire layers at the same time. MSLA is a balanced approach by considering the combined effect with respect to print speed, accuracy and resolution [25]. Such a method takes into account high SLA resolution and DLP efficiency as a versatile printing option for widespread applications [16]. MSLA yields good mechanical properties in a comparable manner to DLP, which is favoured for both professional and hobbyist use owing to its cost-effectiveness and easy maintenance. Among key strengths with respect to VP, it is worthwhile to highlight its high resolution, good reliability and design flexibility as a preferred option to create complex and stable architecture with various material formulations such as hydrogels, elastomers, composites and biological materials [8,26]. This method is instrumental in advanced development of soft sensors or actuators and bionic adhesive devices, resulting in the versatility of producing innovative and functional objects [26,27].

VP has also a major application in the medical field to focus on 3D printed biodegradable medical devices using emerging photopolymerisation [28]. It is also well utilised to assess the impact on mechanical and biological properties of 3D printed denture bases with an emphasis on dental applications [15]. Other applications can expand to drug delivery systems and the fabrication of ceramic bodies without warping with great potential in diverse fields [29–31]. The ability of VP techniques to work with various materials, including nanocomposites or nanofibre-reinforced composites [8,26], is crucial for particle-reinforced resin composites. This versatility allows for incorporating diverse types and sizes of reinforcing particles, potentially leading to a wide range of achievable mechanical properties. When predicting mechanical properties of particle-reinforced composites, it is essential to consider specific VP techniques used as follows:

- SLA offers high accuracy and smooth surfaces [15,22], which may influence particle distribution and interface quality in composites.
- DLP provides higher mechanical strength and stress resistance compared to SLA [19], which is potentially beneficial for particle-reinforced composites with enhanced durability.
- MSLA balances print speed, accuracy and resolution [25], which could affect overall quality and consistency of particle-reinforced composites.

Understanding these technique-specific characteristics is crucial for developing accurate predictive models, particularly used for mechanical properties of 3D printed particle-reinforced resin composites.

As far as material properties are concerned, VP enables the creation of tough and resorbable networks, and further enhances material dispersion like hydroxyapatite whiskers for better mechanical performance used for orthopaedic applications [32]. Such a method is also widely used to produce polyurethanes requiring specific viscosities to achieve optimal print resolution [33]. On the other hand, VP can be integrated into developing advanced energy solutions like recyclable 3D printed lithium-ion batteries with its major adaptability to different innovative technologies [34]. When compared with other 3D printing techniques, VP benefits from its high print resolution, quick print time and cost-effectiveness in manufacturing equipment and materials [35].

The incorporation of particles as reinforcements in resin matrices offers a great opportunity to enhance mechanical properties of 3D printed parts [36]. However, predicting the mechanical behaviour of composite materials remains a significant challenge due to complex interactions between reinforcing particles, resin matrices and processing parameters used in 3D printing [37].

Accurate prediction of mechanical properties is vital for optimising material formulations and printing parameters to achieve desired performance characteristics in final products. Conventional approaches to property prediction often rely on empirical models or finite element analysis (FEA), which may not fully capture the multifaceted nature of 3D printed particle-reinforced composites [38,39]. However, recent advancements in modelling techniques, including the integration of artificial intelligence (AI) and machine learning algorithms, offer a promising means for improving the accuracy and reliability of mechanical property predictions [40,41]. These approaches can potentially account for nonlinear effects of particle reinforcement, processing parameters and material-specific characteristics that significantly influence final properties of 3D printed composites [42].

Material innovation with enhanced mechanical properties is critical to meet such challenges associated with the widespread adoption of DLP at an industrial level [3,24,43]. Mechanical strength, toughness and overall material performance of 3D printed parts can be improved when incorporated with different types of particles as additives within resin matrices in a composite system [44,45].

The fusion of empirical models and AI models facilitates the optimisation of material formulations for specific applications by providing predictive insights into mechanical performance of particle-reinforced resin composites [46]. Engineers and designers can utilise these predictive models to iteratively refine material compositions, fine-tune processing parameters, and optimise structural designs. This iterative optimisation process enables the tailored engineering of 3D printed parts with predetermined mechanical properties, thereby accelerating innovation and product development cycles.

This review aims to critically examine fundamental approaches to predicting mechanical properties of 3D printed particle-reinforced resin composites, with a major focus on DLP technology. In particular, conventional composite theory, empirical modelling techniques, and the emerging role of AI in enhancing predictive capabilities have been holistically covered. By investigating mechanisms, advancements, limitations and feasibility of various predictive methods, it offers clear insights into optimising material selection and processing parameters for improved mechanical performance of 3D printed particle-reinforced resin composites.

# 2. Predictive Methods

The existing literature on predicting mechanical properties of 3D printed particlereinforced resin composites reveals several inconsistencies, particularly in the scope and depth of reviews, methodological approaches and integration of advanced technologies [47,48]. While the field benefits from diverse methodologies, the lack of standardised testing and critical comparison between methods obstructs the ability to draw comprehensive conclusions [49]. Data quality and sharing issues further complicate this, leading to the variability in reported results. Moreover, inconsistent applications of AI and machine learning techniques, as well as limited practical implementation, highlight an evident gap between theoretical advances and real-world applications [49,50]. Finally, the scalability and practical relevance of predictive models, as well as their validation and accuracy, remain significant challenges [51]. Addressing these inconsistencies through more rigorous, standardised and integrative research approaches can enhance predictive modelling of mechanical properties in 3D printed composites, thus bridging the gap between academic research and industrial commercialisation.

Several studies have utilised different mathematical models to investigate mechanical properties of 3D printed composites. Kang et al. [52] employed microscopic models by varying diameters and dispersity of hydroxyapatite (HA) particles to estimate mechanical properties via FEA in 3D printed polyether ether ketone (PEEK)/HA composite filaments using fused deposition modelling (FDM). It has been found that the Halpin–Tsai model is very useful for accurately predicting the relationship between elastic modulus and volume fraction of the fillers using an empirical parameter, as seen in Figure 2 [52]. Furthermore, Hetrick et al. [53] used micromechanical models to predict mechanical properties of additively manufactured composites reinforced with continuous carbon fibres (CFs), which concentrated on significant impact of fibre content in these models. Voigt model [53,54]

has been shown to accurately predict longitudinal tensile strength, but reasonably estimate longitudinal modulus at different fibre contents. It is worth mentioning that Ruess model [53,54] may fail to capture estimated transverse modulus for transverse properties of composites, as opposed to Halpin-Tsai model, offering a better fit with the incorporation of more experimental parameters. The addition of fibres in 3D printed composite materials could decrease transverse strength, which is similar to conventional composites. Additionally, transverse strength could diminish with increasing fibre volume fraction.

Nonetheless, the change in shear modulus with the variation of fibre content cannot be adequately modelled simply by using either Halpin-Tsai model or Reuss model. Halpin-Tsai model, while flexible, often requires the calibration against experimental data to provide accurate predictions for specific composite systems. This calibration process can be time-consuming and may not generalise well across varied materials and printing parameters. Reuss model tends to underestimate the transverse modulus of composites, particularly for 3D printed materials with complex fibre orientations and distributions. Both models assume idealised fibre arrangements and perfect bonding between fibres and matrices, which may not reflect the reality of 3D printed composites.



**Figure 2.** (a) The minimum and maximum elastic moduli for different material formulations of PEEK composites; (b) the coefficient of anisotropy compared to different composite formulations; (c) data comparison with respect to elastic modulus between experimental data and numerical results for different composite formulations and (d) Halpin–Tsai model for effective elastic moduli of composite materials [52].

The interface between resin matrices and filler particles is very important in determining overall mechanical properties of 3D printed resin composites [55]. Strong chemical bonding at the interface is essential for effective stress transfer from the matrices to reinforcing particles, ultimately enhancing the strength, stiffness and toughness of composites [56]. The acid–base theory developed by Fowkes [57] is useful to better understand filler–matrix interactions in composites, and evaluating acid–base characteristics of different resins and fillers can guide the selection of compatible materials for optimal composite properties. Such interactions are significant in adhesion, surface chemistry and interfacial bonding [55,58]. Custom coupling agents enable to be developed or selected based on specific acid–base characteristics of the resin and fillers to maximise interfacial adhesion, such as silane coupling agents that mediate the interface between organic polymers and inorganic fillers, along with the formation of covalent bonds for both phases [55]. Strong chemical bonding at the interface can improve long-term durability and environmental resistance of 3D printed composite parts, and thus the strength of adhesive bonds is directly related to the change in exothermic interfacial energy, which can be enhanced by acid–base bonding [56]. Chemical coupling agents and surfactants significantly affect interphase dielectric constant of polymer/ceramic composites [59]. These concepts are associated with

influence adhesive interactions with tooth tissues [60]. Several well-established models have been developed to predict the behaviours of 3D printed composites, which are based on well-known classical composite theory discussed in the forthcoming sections.

diverse applications, as exemplified by dental polymers, where their acid-base properties

#### 2.1. Mori-Tanaka Model

Mori–Tanaka model is a micromechanical model often used to predict effective mechanical properties of composite materials. This model is used to analyse 3D printed resin composites via DLP [61,62]. Theoretical equations of Mori–Tanaka model depend primarily on different composite types such as fibre-reinforced composites, particulate composites, laminate composites, etc.

In particular, Mori–Tanaka model is quite beneficial to homogenising materials with complex microstructures in composite materials. With the inclusion of recycled particulates into 3D printed resin matrices, Mori–Tanaka model assists in effectively homogenising such materials for a reasonable prediction of their overall mechanical properties of resulting composite materials [63]. This model takes into consideration specific microstructures of reinforcements and matrices, including a series of parameters such as reinforcement shape and size, as well as orientation distribution [64]. The downside aspect of using Mori–Tanaka model lies in the assumption of simplified reinforcement geometry relative to more irregular shapes of milled resins in practice [65]. More importantly, interfacial adhesion has not been thoroughly considered between reinforcements and matrices, which is crucial in the analysis of 3D printed composites in terms of reinforcement efficiency. This model is limited only to a linearly elastic behaviour. As such, it may not capture full complexity of composite material characteristics when reinforced with irregular particles.

The mathematical formula with respect to Mori–Tanaka model represents effective stiffness tensor of composites, as shown in Equation (1)

$$C^* = C_m + f(C_p - C_m)A[(1 - f)I + fA]^{-1}$$
(1)

where  $C_m$  and  $C_p$  refer to stiffness tensors of the matrix and particles respectively. f is the volume fraction of particles, I is the fourth-order identity tensor, and A is strain concentration tensor of a single particle in an infinite matrix. A is given by Equation (2) below

$$A = \left[I + S(C_m)^{-1}(C_p - C_m)\right]^{-1}$$
(2)

where S is Eshelby tensor, depending on particle shape and matrix properties.

Key assumptions of Mori–Tanaka model include uniform particle distribution throughout the matrix, linear elastic behaviour of both the matrix and particles, perfect particle– matrix bonding, and relatively low particle concentrations [66]. The model also assumes ellipsoidal inclusions within typically an isotropic matrix material. While such assumptions enable Mori–Tanaka model to provide accurate predictions for many composite systems, they may limit its applicability in high particle concentrations, irregular particle shapes, or significant interfacial effects. Despite these disadvantages, Mori–Tanaka model remains a valuable theoretical modelling tool for initial property prediction and material design optimisation in particle-reinforced composites, including those produced via DLP.

#### 2.2. Eshelby Model

Eshelby model applies to predicting the stress and strain fields within a heterogeneous material containing inclusions such as particles, fibres or voids embedded within a matrix [61,62]. This model assumes that inclusions and the matrix possess different mechanical properties. When used in conjunction with Mori–Tanaka model, it analyses composite materials by considering milled resin particles as the inclusions within the resin matrix. It predicts the effective elastic properties of resulting composites based on constituent properties and their volume fractions.

Eshelby model can handle more complex inclusion shapes than Mori–Tanaka model based on simplified geometries, potentially better representing irregular milled resin particles [61]. It inherently accounts for the interaction between the inclusion and the surrounding matrix using Eshelby tensor, which provides a more rigorous process of stress transfer [61,62].

However, this model depends primarily on idealised inclusion shapes, which might only partially capture actual particle morphology. It primarily focuses on linearly elastic material behaviour, thus potentially limiting its applicability to such materials with nonlinear responses or structural damage due to the recycling process. While Eshelby model offers a more sophisticated approach than Mori–Tanaka model for certain aspects, like handling complex inclusion shapes and stress interactions, its limitations and inherent challenges for modelling recycled resin composites necessitate careful consideration and potential adaptation.

Eshelby model is useful for advancing our understanding and optimising 3D printed resin composites, especially those modified with additives [61]. This analytical approach is pivotal for dissecting stress distribution within heterogeneous materials, which further promotes a deeper understanding of how stress is effectively transferred and distributed throughout a composite structure by examining the filler–matrix interaction [62,67]. This mechanism is fundamental to predicting failure mechanisms and assessing overall mechanical performance of composite materials. These factors are crucial as they directly influence the mechanical properties of composites, including stiffness, strength and ductility. By applying Eshelby model, researchers and engineers can evaluate how the variations in these geometric parameters impact mechanical performance of resulting composite materials.

Additionally, the volume fraction of inclusions emerges as a critical parameter within this analytical framework [67]. The inclusion of additives alters the volume fraction of reinforcements within the matrix, thus significantly influencing the properties of composite materials. With the aid of Eshelby model, it is much easier to understand and predict how changes in the volume fraction of inclusions influence the mechanical behaviour of composite materials. This predictive capability is invaluable for developing and refining composite materials used in 3D printing, which further enables to create specific resin composites with well-tailored properties for widespread applications.

#### 2.3. Halpin–Tsai Model

Halpin–Tsai model is well recognised as a theoretical framework designed to estimate mechanical properties of composite materials, with a specific focus on fibre-reinforced composites according to Luo et al. [68] and Martinez-Garcia et al. [66]. Halpin–Tsai model establishes a correlation between mechanical properties of composite materials (e.g., elastic modulus and strength) and the characteristics of corresponding constituents such as re-inforcing fibres and the matrix. The major application of Halpin–Tsai model lies in their utilisation to determine elastic modulus (known as stiffness) of composite materials. This determination is useful to analyse volume fraction and inhere properties of reinforcing fibres and matrix [66,69]. Furthermore, Halpin–Tsai model can be modified to account for various material conditions, including isotropic and anisotropic states, as well as to accommodate different loading conditions, according to Fuchs et al. [70]. This versatility makes Halpin–Tsai model an invaluable analytical framework in predictive analysis and

This model incorporates a comprehensive assessment of orientation, aspect ratio and mechanical characteristics of reinforcing fibres, along with the dynamics of their interaction with the matrix [70]. It facilitates a quantitative evaluation of the impact of incorporating reinforcing fibres on mechanical properties of composite materials. Within the scope of 3D printed epoxy composites, Halpin–Tsai model emerges as a predictive tool to characterise the reinforcement effect of fillers or fibres such as carbon and glass fibres or nanoparticles on mechanical performance of 3D printed parts according to Martinez-Garcia et al. [66]. By varying volume fractions and properties of reinforcing fillers, mechanical properties of 3D printed parts can be customarily tailored in order to meet end-user applications. This customisation enables composite materials to meet desired performance criteria such as higher stiffness and strength, and further enhanced impact resistance in order to optimise 3D printed parts for specific applications.

Halpin-Tsai model emerges as a pivotal analytical tool with the consideration of the orientation of reinforcing fibres or particles in a composite material, which is essential for 3D printing of resin composites. This method is particularly utilised for understanding the impact that the orientation of recycled particulates has on overall mechanical behaviour of resulting composites [70]. Similar to other analytical approaches, Halpin–Tsai model offers an effective approach to account for volume fraction of reinforcing phase within composites. The variation of volume fraction allows for investigating the influence of recycled milled powder resin content on mechanical properties of composite materials, such as stiffness, strength and toughness [66]. Furthermore, Halpin–Tsai model incorporates special considerations for aspect ratio of reinforcing phase, which is crucial to better understand how the shape and size of recycled milled resin particles affect mechanical properties [68]. In general, aspect ratio influences the efficiency of reinforcements, which also plays a significant role in determining the performance of composite materials. As such, this approach facilitates a nuanced understanding of how orientation, volume fraction and aspect ratio of reinforcing phase impact mechanical performance of composite materials, which is vital in the development and optimisation of 3D printed resin composites.

Empirical Halpin–Tsai model is primarily derived from experimental data, which is opposed to Mori–Tanaka model and Eshelby model based on theoretical principles from mechanics of materials [70]. Halpin–Tsai model is particularly applicable to fibre-reinforced composites, while Mori–Tanaka model and Eshelby model expand to various types of composite materials and microstructures [61,62]. Eshelby model typically involves complex mathematical formulations and calculations when compared with more straightforward Halpin–Tsai model and Mori–Tanaka model.

Researchers have investigated the use of modified Halpin–Tsai model to predict mechanical performance in polymer nanocomposites reinforced with spherical fillers [66,68]. The mathematical model proposed by Martinez-Garcia et al. [66] considered combining a three-phase framework and fundamental percolation concepts, glassy layer and colloidal glass transition into a cohesive analytical tool. Such a model represents the evolution of a three-phase series-parallel model initially developed by Ji et al. [71], which was further refined by the percolation theory aforementioned by Schilling et al. [69]. Such advances shed light on the prediction of mechanical properties of polymer nanocomposites reinforced with spherical nanoparticles.

Martinez-Garcia et al. [66] created a more complex equation to estimate tensile modulus with the inclusion of spherical nanoparticles. In particular, Equations (3)–(5) consider moduli of composites and polymer matrix, volume fraction of particles, as well as critical percolation threshold. It can combine particle interaction and percolating network very well as an advanced approach to predict tensile properties of polymer nanocomposites.

$$E_{c} = E_{m} \left[ (1-\delta) + \frac{\delta - \gamma}{(1-\delta) + \left(\frac{k-1}{\ln(k)}\right)\gamma + \left(\left(k + \frac{\sqrt{2}}{2}(k-1)\right)(\delta - \gamma)\right)} + \frac{\gamma}{(1-\delta) + \frac{(\delta - \gamma)(k+1)}{2} + \gamma\frac{E_{f}}{E_{m}}} \right]$$
(3)

$$\delta = \begin{cases} 0 & : 0 \le \phi \le \phi_p \\ \sqrt{\left(1 + \frac{r}{R}\right)\phi_g\left(\frac{\phi - \phi_p}{\phi_g - \phi_p}\right)^{\frac{\alpha}{2}}} & : \phi_p < \phi \le \phi_g \end{cases}$$
(4)

$$\gamma = \begin{cases} 0 & : 0 \le \phi \le \phi_p \\ \left[ \sqrt{\phi_g} \left( \frac{\phi - \phi_p}{\phi_g - \phi_p} \right) \right]^{\frac{\alpha}{2}} & : \phi_p < \phi \le \phi_g \end{cases}$$
(5)

where  $E_c$  denotes the tensile modulus of composite materials, which is a primary output of the model. It also represents the stiffness of composite materials, which is influenced by the distribution of nanoparticle fillers within polymer matrices.  $E_m$  is tensile modulus of polymer matrices to denote inherent stiffness of neat polymer without any reinforcements.  $\delta$  is a dimensionless parameter with respect to volume fraction of particles within composite materials. It can be defined in terms of particle radius R, interphase thickness r, volume fraction of glassy phase  $\varphi_{g}$ , as well as percolation threshold  $\varphi_p$ .

The model can be modified by such a parameter to account for an effective particle contribution to the stiffness of composites, particularly above their percolation threshold, shown in Figure 3 with a variety of composites.  $\gamma$  is another dimensionless parameter in relation to volume fraction of particles to focus on particle contribution to volume fraction of glassy phase transition within the specific range of percolation threshold. Tensile modulus of fillers  $E_f$  represents the stiffness of nanoparticles, which is essential to understand intrinsic properties of fillers with the impact on overall composite stiffness.  $\varphi$ ,  $\varphi_p$  and  $\varphi_g$ denote volume fraction of particles, percolation threshold and glassy phase volume fraction respectively.  $\varphi$  represents nanoparticle concentration in composite materials. Additionally,  $\varphi_p$  is the critical concentration in which a significant increase in mechanical properties takes place due to the formation of a percolating network. On the other hand,  $\varphi_g$  is the concentration at which the system transitions into a glassy state, which is deemed the maximum effective filler concentration for mechanical reinforcement. Percolation exponent  $\alpha$  influences the prediction of mechanical reinforcement based on particle aggregation dynamics and the formation of interphase glassy state. As such, it offers great insight into close filler-matrix interaction and sophisticated development of percolating networks.

Interface modulus ratio, also known as *k*-parameter, represents relative stiffness of interphase area when compared with that of polymer matrices. It is a key factor for the measurement of reinforcement effectiveness induced by interphase areas surrounding nanoparticles. Chemical interactions, particularly those facilitated by coupling agents like  $\gamma$ -aminopropyltriethoxysilane ( $\gamma$ -APS), significantly influence this parameter, and thereby overall reinforcement effectiveness [72].  $\gamma$ -APS improves the interfacial adhesion between the matrices and reinforcing particles or fibres, particularly as evidenced by covalent bonds with both glass fibres and polymer matrices to create a strong interphase region [72,73]. This enhanced adhesion is reflected in a higher *k*-parameter value. Silane groups in  $\gamma$ -APS can form covalent bonds between inorganic filler surfaces and organic polymer matrices, leading to a strong chemical linkage at the interface. Higher *k*-parameter values can also be substantiated due to stress transfer efficiency, modification of interphase region and surface energy and reduction of interfacial defects [74–76].



**Figure 3.** Young's modulus versus theoretical prediction of (**a**) polyolefin/carbon black composites, (**b**) polyolefin/fumed silica composites, (**c**) PEEK/Al<sub>2</sub>O<sub>3</sub> composites, (**d**) PEEK/SiO<sub>2</sub> composites, (**e**) PTMHMTA/TiO<sub>2</sub> composites and (**f**) P(MMA-MTC)/SiO<sub>2</sub> composites. Red squares denote experimental results. Equation (1), (solid blue line), Ji model (brown dashed line), Guth–Smallwood–Einstein model (pink dashed line), Kerner model (green dashed line) and Halpin–Tsai model (black dashed line) [66].

Different coupling agents can be used to tailor the properties of interphase region. For instance,  $\gamma$ -APS might create a different interphase than other silanes [77]. This tailoring ability allows fine-tuning of *k*-parameter to optimise specific mechanical properties. Chemical interactions facilitated by coupling agents can influence dynamic mechanical response of composites [78]. This response can be reflected in factor-dependent *k*-parameter in relation to strain rate or temperature for a complex viscoelastic behaviour at the interface [75]. Coupling agents improve environmental resistance of the interface, and further maintain reinforcement effectiveness over time under various conditions [75].

The model developed by Martinez-Garcia et al. [66] comprises several pivotal elements used in mechanical reinforcement of polymer composites, which mainly focuses on certain aspects to contribute to a better understanding towards material behaviour of composites. First of all, it enables to identify percolation volume fraction  $\varphi_p$  above which reinforcing

particles within composite materials generate a percolating network for the stepwise improvement of mechanical properties. This network can be affected by a variety of factors, including particle size, shape and orientation, along with the interphase of these particles.

In addition, this model integrates the concept of colloidal glass transition into its framework, which indicates a particular state where particle movements within composites may decelerate significantly and virtually halt. This depends primarily on particle concentration within composite materials. Glass transition plays a vital role in accurately characterising mechanical performance of composite materials, which is considered as critical phase behaviour for overall material characteristics. Furthermore, critical percolation exponent was developed by Martinez-Garcia et al. [66] as a key parameter in this model to explore aggregation dynamics of particles and the rapidity with which interphase glass state induces. This exponent can directly benefit the establishment of an intricate relationship between particle interaction and their joint impact on mechanical reinforcement of composite materials. Such model components all together provide a comprehensive approach to holistically assess mechanical performance of polymer composites, thus elucidating a complicated relationship between microstructures of composites and mechanical properties on the macroscale. This comprehensive approach is validated with experimental data from six polymer nanocomposites, including nanofillers in size of 15-30 nm,  $Al_2O_3$ and  $SiO_2$ , reinforcing PEEK composites, which demonstrates a good agreement between theoretical prediction and experimental data for their enhanced mechanical properties. The modelling ability to accurately evaluate mechanical reinforcement of nanocomposites highlights exciting potential for material design with optimal mechanical performance for diverse technological applications.

On the other hand, Luo et al. [68] proposed the combination of the rule of mixtures (ROM) [79] and Halpin–Tsai model to precisely estimate tensile strength and Young's modulus of epoxy composites reinforced with microsized CFs, rubber nanoparticles (RNPs) and carbon nanotubes (CNTs) via fused filament fabrication (FFF). A reduction factor has been incorporated to address the nonlinear behaviour of tensile strength with respect to fibre volume fraction based on modified ROM. Halpin–Tsai model has also been modified to achieve more accurate predictions of mechanical properties with multiscale reinforcements. Such a variation in analytical and empirical modelling approaches considers a distinct contribution made by each type of reinforcements to the overall modulus of composite materials. The robustness and reliability of such modified models can be further proven by experimental validation with synergetic effect induced by the incorporation of multiscale reinforcements. Such synergetic effect is vital to significantly improve mechanical strength and toughness of composite materials, which highlights the applicability of such models in the optimisation of composite materials via FFF. Luo et al. [68] developed an effective modelling approach to deal with complex micro/nanostructures of composite materials, as well as interactions between the matrix and multiscale reinforcements. Equation (6) represents Young's modulus  $E_c$  of a composite material, considering the volume fraction  $\varphi_{RNP}$  and the modulus of RNPs  $E_{RNP}$ , along with an interphase effect where  $\varphi_{int}$  and  $E_{int}$ refer to volume fraction and Young's modulus for the interphase respectively. This accounts for unique interfacial properties between the matrix and surrounding nanoparticles. This equation is especially useful to understand how micro/nanoscale modification impacts mechanical properties of resulting composite materials at a macroscopic level.

$$\frac{E_c}{E_{m_2}} = \frac{1 + 2\eta_{RNP}\varphi_{RNP} + 2\eta_{int}\varphi_{int}}{1 - \eta_{RNP}\varphi_{RNP} - \eta_{int}\varphi_{int}}$$
(6)

Equation (7) defines a parameter  $\eta_{RNP}$ , which can be used to correlate elastic modulus of RNPs  $E_{RNP}$  and elastic modulus of the matrix  $E_{m2}$ . This equation elaborates how reinforcement effect of nanoparticle impact overall stiffness of composite materials.

1

$$\eta_{RNP} = \frac{E_{RNP}/E_{m_2} - 1}{E_{RNP}/E_{m_2} + 1}$$
(7)

Equation (8) defines a parameter  $h_{int}$ , used to correlate interphase modulus  $E_{int}$  to matrix modulus  $E_{m2}$ , which reveals the significance of interphase properties to tailor mechanical behaviour of composite materials.

$$\eta_{int} = \frac{E_{int}/E_{m_2} - 1}{E_{int}/E_{m_2} + 1}$$
(8)

Equation (9) defines interphase volume fraction  $\varphi_{int}$  by incorporating nanoparticle radius *R* and interphase thickness *R<sub>i</sub>* in order to quantify important filler–matrix interactions.

$$\varphi_{int} = \left[ \left( \frac{R + R_i}{R} \right)^3 - 1 \right] \varphi_{RNP} \tag{9}$$

Finally, Equation (10) based on modified Halpin–Tsai model is used to predict elastic modulus of multiscale composite materials reinforced with CFs and CNTs with the consideration of effect of RNPs and interphase. In particular, the subscript L represents the longitudinal direction in alignment with the fibre orientation to significantly affect the stiffness of composite material. Whereas, the subscript T denotes the transverse direction (i.e., perpendicular to the fibre direction).

$$E_{c} = E_{m0} \times \left[\frac{3}{8} \left(\frac{1 + \xi_{CF} \eta_{CF_{L}} \cdot \varphi_{CF}}{1 - \eta_{CF_{L}} \cdot \varphi_{CF}}\right) + \frac{5}{8} \left(\frac{1 + 2\eta_{CF_{T}} \cdot \varphi_{CF}}{1 - \eta_{CF_{T}} \cdot \varphi_{CF}}\right)\right] \times \left[\frac{3}{8} \left(\frac{1 + \xi_{CNT} \eta_{CNT_{L}} \cdot \varphi_{CNT}}{1 - \eta_{CNT_{L}} \cdot \varphi_{CNT}}\right) + \frac{5}{8} \left(\frac{1 + 2\eta_{CNT_{T}} \cdot \varphi_{CNT}}{1 - \eta_{CNT_{T}} \cdot \varphi_{CNT}}\right)\right] \times \left[\frac{1 + 2\eta_{RNP} \cdot \varphi_{RNP} + 2\eta_{int} \cdot \varphi_{int}}{1 - \eta_{RNP} \cdot \varphi_{RNP} - \eta_{int} \cdot \varphi_{int}}\right]$$
(10)

Based on this modelling approach, Luo et al. [68] shows in Figure 4 that with constant CFs (10 phr) and RNPs (4 phr), the relative error between experimental and theoretical values is over 10% at the CNT contents of 0 and 0.25 phr. However, as CNT content increases to 0.5, 0.75 and 1 phr, these errors decrease to 5% or less, resulting in better model accuracy. The higher initial errors suggest that at a low CNT content, the bonding between reinforcements and resin matrices is imperfect. The interfacial bonding is enhanced with increasing CNT content. However, at the CNT content of 1 phr, the relative error appears to increase again due to filler reaggregation at higher CNT contents.



**Figure 4.** Experimental and theoretical comparison showing increasing errors for elastic modulus with decreasing CNT content [68].

Yang et al. [45] introduced a mathematical model to correlate the degree of cure with tensile strength and hardness of materials fabricated via SLA. This model effectively quantifies the solidification stages of both initial green parts and those under UV post-curing

process, thereby facilitating a high degree of predictive accuracy with respect to mechanical properties of photosensitive liquid resins. The model can accurately estimate tensile strength and hardness by integrating a range of parameters, including layer thickness, stratification angle and curing duration, as supported by an explicit solution algorithm [45]. Predictive precision is exemplified by average accuracies of 88% and 90% for tensile strength, as well as 98% and 95% for hardness with respect to green and UV post-cured parts respectively. UV post-curing process is identified as a significant enhancer of mechanical performance, with a key emphasis on valuable applications of the model in the refinement of AM processes.

The accuracies of Mori–Tanaka model, Eshelby model and Halpin–Tsai model vary to a different extent, depending on specific composite systems and predicted properties. Mori–Tanaka model provides good accuracy for a wide range of particle volume fractions. For instance, Gupta et al. [61] reported an excellent agreement with experimental data for fibre-reinforced polycarbonate composites up to moderate volume fractions ( $\leq 10$  vol%). Eshelby model is highly accurate for dilute concentrations of inclusions but may lose the accuracy at higher volume fractions [61,62]. Wong et al. [62] demonstrated that Eshelby model is particularly precise for predicting effective stiffness of composites with spherical inclusions at low concentrations. Halpin–Tsai model with its simplicity offers reasonable accuracy, especially for fibre-reinforced composites. Paspali et al. [80] showed that Halpin–Tsai model induced good predictions for tensile and flexural moduli of PLA/organoclay composites with the inclusion of 1 and 5 wt% organoclays.

The above-mentioned three models exhibit diverse levels of computational complexity. Mori–Tanaka model yields moderate complexity with the requirement of tensor calculations despite being generally less computationally intensive than full numerical simulations [62]. Eshelby model, on the other hand, has higher complexity due to the requirement to calculate Eshelby tensor, which appears to be challenging for non-ellipsoidal inclusions [62]. Halpin–Tsai model has low complexity instead with its semi-empirical nature to make it computationally efficient and easy to implement [68].

Each model has its specific strengths regarding the applicability to different composite types and loading conditions. Mori–Tanaka model is well-suited for particulate composites and short-fibre composites, enabling it to handle multiple phases and orientations, which is effective for both elastic and thermoelastic properties [61]. Eshelby model is ideal for ellipsoidal inclusions in an infinite matrix, which can be further extended to handle multiple inclusions and orientations despite its complexity [67]. It is primarily used for elastic properties. Halpin–Tsai model, originally developed for fibre-reinforced composites, has been adapted for particulate composites as well [81]. It is best suited for unidirectional loading conditions, which can be inadequate in complex 3D stress states.

Model selection for 3D printed particle-reinforced resin composites depends on specific characteristics of diverse composite systems. Halpin–Tsai model may provide a good balance of accuracy and computational efficiency for particular composite systems with low to moderate particle concentrations and simple geometries. Mori–Tanaka model might offer better accuracy, notwithstanding increased computational cost for composites in possession of higher particle concentrations or more complex particle shapes. Eshelby model could be particularly useful in the case that a detailed analysis of stress concentration around individual particles is required. However, it may be overly complex for routine property predictions.

#### 2.4. Other Models

Moghadasi et al. [82] developed a computational fluid dynamics (CFD) model for top-down DLP to predict the DLP-based resin behaviour in 3D printing. This model helped to analyse the effects of various process parameters, including fluid viscosity, travelling speed, travelling speed ratio, printed layer thickness, and travel distance on the stability time of the resin. The stability time is critical since it indicates the duration necessary for the resin to stabilise after each layer is printed, which impacts overall print quality and efficiency. The model utilised mass and momentum conservation equations for an incompressible Newtonian fluid. These equations help calculate the fluid dynamics for DLP, in which the resin flow should be precisely controlled. A 2D simulation environment using FLOW-3D software v12 update 3 was then employed, which was known for its capability to handle complex fluid dynamics simulations. The equations can be solved using a second-order accurate scheme for space and an implicit method for time, thus ensuring numerical stability and accuracy. Through this modelling, the following key points can be summed up:

- Higher viscosity leads to longer stability time, indicating that the resin takes longer time to stabilise, which can slow down 3D printing processes.
- Increasing travelling speed reduces stability time with the potential for faster printing cycles.
- The variations in travelling speed ratio have less impact on stability time than other parameters.
- Thicker layers result in shorter stability time, which could give rise to faster printing, but may compromise fine details and accuracy in 3D printing.
- Larger travel distance increases stability time, which suggests that the resin requires more time to stabilise, potentially slowing down 3D printing processes as well.

Setter et al. [83] effectively evaluated, selected and advanced kinetic modelling procedures for UV-curable acrylates in multiphoton lithography and fusion jetting based on Kamal-Sourour equation. Initially, various models were analysed using UV-DSC measurements through single and clustered measurements. The analysis of single measurements showed that most selected models could achieve acceptable fit accuracy, while Kamal– Sourour and Avrami methods yielded the best results [83,84]. Kamal–Sourour method, in particular, accurately captured the sigmoidal aspect of curing reaction in support of the theory of a combined autocatalytic and *n*-th order reaction. This method demonstrates that reaction orders are proportional to UV intensity, but can be independent of isothermal temperature.

Conversely, Avrami method shows that reaction orders increased with UV intensity, thus approximately leading to a limited growth function. Kamal–Sourour method was selected for subsequent modelling based on its higher coefficients of determination and greater chemical plausibility, as seen in Figure 5. Two clustering strategies, namely UV-intensity-based and temperature-based strategies, were analysed to support temperature independence of reaction orders. The clustered analysis demonstrated the exponential decay of reaction orders with increasing UV intensity, which is consistent with single measurement analysis results. Overall, the model achieved higher mathematical determination for all kinetic parameters, allowing for isothermal predictions at unmeasured UV intensities. The calculated progression matched those measured UV-DSC data, with kinetic parameters showing near-linear changes with increasing the temperature. The model involves reaction rate constants and reaction orders, which depend on the reaction conditions like temperature *T* and UV intensity *I*. Equation (11) represents this model as given below:

$$\frac{d\alpha}{dt} = k_1 \cdot (1-\alpha)^{n_{gen}} + k_{cat.gen} \cdot k_2 \cdot \alpha^{m_{gen}} \cdot (1-\alpha)^{n_{gen}}$$
(11)

where  $\alpha$  is the degree of cure,  $k_1$  and  $k_2$  are the reaction rate constants for the *n*-th order and autocatalytic reactions respectively, and  $n_n$  and  $m_m$  are the reaction orders associated with these processes.



**Figure 5.** The relationship between UV intensity, temperature, and curing kinetics of acrylate A. (**A**) a chemical structure of dimethacrylates and diacrylates used as key building blocks in acrylate A and acrylate B, and (**B**) curve-fitting results of various kinetic models used to describe the curing reaction of acrylate A under a UV intensity of 7.5 mW/cm<sup>2</sup> at the constant temperature of 30 °C (Fit quality is indicated by the coefficient of determination), and (**C**) kinetic predictions for acrylate A at 90 °C under UV intensities of 40 and 90 mW/cm<sup>2</sup>, based on the enhanced Kamal–Sourour equation in comparison with those predictions with actual UV-DSC measurements [83].

Redmann and Osswald [85] introduced a phenomenological model to track and predict modulus development of dual-cure resin systems under thermal processing. Dual-cure systems, which involve both UV and thermal curing processes, exhibit unique behaviours when compared with conventional thermosetting resins due to their two-stage curing reaction. This model is significantly important because it addresses the nonlinear development of elastic modulus in such systems. It particularly focuses on the observable softening effect and high potential for large structural deformation when the processing temperature exceeds  $T_g$  of intermediately cured material. The model defines the modulus as a function of temperature difference relative to  $T_g$ , which is expressed in Equation (12) as follows:

$$E = \frac{E_G - E_R}{1 + e^{k[T - \lambda(\frac{c(Tg_1 - Tg_0)}{1 - (1 - \lambda)c}) + Tg_0]}} + E_R$$
(12)

where  $E_G$  and  $E_R$  are the moduli at the upper glassy and lower rubbery plateaus respectively. k is a parameter controlling the shape of the modulus transition curve.  $\Delta T$  is the difference between the processing temperature and  $T_g$ .

The model incorporates an empirically derived relationship between  $T_g$  and the degree of cure *c*. In this way, it facilitates a comprehensive understanding of the variation of  $T_g$  with the curing progress. The relationship is further established using Equation (13) as follows:

$$T_g = \lambda \left( \frac{c(Tg_1 - Tg_0)}{1 - (1 - \lambda)c} \right) + T_{g0}$$

$$\tag{13}$$

where  $\lambda$  is a parameter indicative of the ratio of heat capacities between fully cured and uncured states.  $T_{g1}$  and  $T_{g0}$  represent the glass transition temperatures of fully cured and initial states, respectively.

This model was validated through experiments measuring the modulus at various stages of thermal curing and processing temperatures. The use of this model allows for a refined understanding of material behaviour in dual cure resin systems under different processing conditions. It provides a valuable tool for engineers and researchers to predict and control mechanical properties of materials subjected to complex curing reactions, thereby optimising manufacturing processes, and further enhancing the quality and reliability of final products.

Yang et al. [45] presented a mathematical model for predicting mechanical properties of photosensitive liquid resins via SLA. The study addresses a typical gap in existing research by linking the degree of cure of the resin to its resulting mechanical properties, such as tensile strength and hardness. The model is developed to estimate the degree of cure for freshly printed (green) and UV post-cured parts. Such a model incorporates layer thickness and stratification angle, influencing how the light interacts with the resin during curing processes. The model is established to predict tensile strength and hardness of fabricated parts by using the degree of cure as a essential parameter. It enables accurate predictions based on the solidification level achieved during and after 3D printing processes. The following lists key points given by

- The study provides a significant tool for manufacturers to predict and optimise mechanical properties of SLA parts by adjusting processing parameters effectively.
- By establishing a direct correlation between the degree of cure and key mechanical properties, the research enhances the structural integrity and functional performance of 3D printed parts.

This research not only fills a crucial research gap by providing a mathematical modelling approach for predicting mechanical properties from the degree of cure, but also supports enhanced industrial applications of SLA for critical material performance.

# 3. Limitations and Gaps

Integrating these methodologies and findings from various AM techniques and modelling approaches can significantly contribute to developing a comprehensive mathematical model used for various particle-reinforced resin composites via DLP. This model would accurately predict mechanical properties and yield 3D printing optimal parameters for enhanced material performance.

The limitations and gaps in current models for 3D printing of epoxy resins using DLP take into account the complexity of 3D printing processes, material behaviour, as well as outcome predictability. Empirical models often struggle with complex chemistry of epoxy resins and dynamic changes during the curing process. Typical variables such as temperature, UV exposure time and resin composition can significantly affect final properties of 3D printed parts [86]. An effective way to overcome this limitation is to develop multiscale models that integrate chemical kinetics with mechanical properties to better predict the behaviour of epoxy resins during and after curing processes. Integrating rheological studies into the model can assist in understanding the flow and curing behaviour under different conditions. By employing advanced material characterisation techniques, such as dynamic mechanical analysis (DMA) and differential scanning calorimetry (DSC), to gather comprehensive data on material properties under various conditions, captured data can be

collected to refine empirical models to more accurately reflect actual material behaviour of epoxy resins. DLP involves intricate processing parameters like light intensity, exposure time and layer thickness that interact in a nonlinear manner. Empirical models may not fully capture these interactions or their impact on mechanical properties and dimensional accuracy of 3D printed objects. Design of experiments (DoEs) is proven to be effective in systematically studying the effects of various printing parameters on the properties of final parts [87]. This method can identify critical parameters and their interactions, along with the provision of a robust dataset for model calibration. Integrated sensors and real-time monitoring systems can capture in-process data, such as temperature gradients and UV exposure levels. Such real-time data can dynamically update the models with improved accuracy and predictive capabilities.

The layer-by-layer fabrication method inherent to DLP yields anisotropy and potential heterogeneities within 3D printed parts. Empirical models often assume homogeneity and isotropy, leading to inaccuracies in material property prediction. Mathematical models can be more accurately formulated by utilising anisotropic material models that account for directional properties of 3D printed parts. These models can be derived from experimental testing of 3D printed samples in different orientations to capture an anisotropic behaviour accurately. By employing microscale modelling techniques, such as FEA at a layer or particle level, we can better understand and predict the effect of heterogeneity within 3D printed parts. These approaches can help identify an optimal print strategy in order to minimise undesired anisotropy.

The microscale features achieved with DLP challenge empirical models, particularly for such parts with intricate geometries or those with the inclusion of nanoparticle reinforcements. The acquisition of these fine details requires high-resolution modelling approaches that can significantly increase computational demands. More accurate models can be formed by adopting a high-resolution modelling technique, such as voxel-based modelling that accurately represents microscale features of DLP-based parts. This approach requires significant computational resources but also offers a more detailed prediction of mechanical properties and surface finish. Moreover, developing a multiscale modelling framework, enabling the connection of high-resolution models at the microscale with coarser models at the macroscale level, can efficiently capture detailed features while providing great insights into overall behaviours of 3D printed parts.

# 4. Theoretical Integration of AI in Mathematical Models

AI tools have significantly enhanced mathematical models in polymer composites, revolutionising this field by enabling more accurate predictions and efficient analyses. One key advancement in this area is the Materials Simulation Toolkit for Machine Learning (MAST-ML), as highlighted by Jacobs et al. [41]. This open-source software package is designed to accelerate data-driven materials research by leveraging machine learning techniques, thereby enhancing the development and optimisation of mathematical models for polymer composites [41]. Moreover, Sharma et al. [46] investigate the advances in computational intelligence specifically tailored for polymer composites. The research discusses critical challenges, such as the curse of dimensionality, overfitting, noise and mixed variable problems, while exploring the latest machine learning algorithms that can be integrated into polymer composites. Recommendations on using various machine learning algorithms to address critical issues in polymer composites offers great insights into potential directions for future research.

Furthermore, Tomás et al. [87] developed a deep neural network for calibrating electrical resistance of self-sensing polymer/CF composites, which is compatible with advanced microprocessor electronics primarily dealing with AI tasks. This innovative approach not only showcases the application of AI in enhancing the sensitivity and calibration of polymer composites but also underscores the importance of nonlinear mathematics in evaluating composite materials, which paves the way for novel methodologies in material science and engineering [87,88]. Additionally, Folorunso et al. [89] emphasised the deployment of flexible and versatile mathematical models for predicting electrical conductivity of polymer composites. By considering the simplicity and adaptability of these models, the research advocates for their optimal utilisation in characterising and simulating electrical properties of polymer composites, which is considered for the pivotal role of AI-driven mathematical models in advancing the understanding and design of polymer composites. They could confirm the weight fraction of fillers with direct impact on electrical conductivity of polymer composites. The incorporation of AI tools in polymer composites has significantly promoted the development and application of mathematical models, which offers researchers innovative avenues to optimise material properties, predict material behaviour, and drive advancements in polymer composites.

Machine learning models have been developed to predict mechanical behaviour of additively manufactured particulate composites, showing excellent agreement with experimental data [90]. The machine learning model developed by Malley et al. [90] was able to accurately predict mechanical behaviour of additively manufactured samples that were physically evaluated with near-unity correlation coefficients. Machine learning model also performed well in predicting the mechanical response of untested, newly formulated material compositions.

The integration of AI and AM has shown the potential to improving efficiency and processability of biocomposites [91]. Verma et al. [91] showed how biodegradable and biocompatible materials could be used as the alternatives to conventional synthetic polymers in composite applications to address environmental concerns. Their use of machine learning and deep learning improved the efficiency and processability of AM methods for biocomposite development.

Hyperparameter tuning is critical in optimising machine learning models for predicting mechanical properties of 3D printed composites [92]. It involves systematically adjusting configuration settings of algorithms to improve their performance and generalisation capabilities [92]. In 3D printed composites, hyperparameters can significantly influence modelling capability to capture complex relationships between printing parameters, material compositions and resulting mechanical properties. Common hyperparameters include learning rate, number of hidden layers in neural networks, number of trees in random forests and regularisation strength. Specific techniques such as grid search [92], random search [93] and Bayesian optimisation [92] are frequently employed to explore hyperparameter space efficiently. For instance, Gu et al. [94] established a deep neural network to predict mechanical properties of carbon fibre-reinforced composites, resulting in a 20% improvement in prediction accuracy when compared with conventional empirical models. This work highlights the potential of advanced machine learning techniques in enhancing predictive capabilities of composite materials. The importance of hyperparameter tuning in this field originates from complex and nonlinear relationships between processing parameters and material properties in AM, in which minor changes in model configurations can yield significant improvements in predictive accuracy.

The optimisation of hyperparameters for machine learning models can be applied to other 3D printed composites as well. For instance, Liu et al. [93] employed a random forest model to predict mechanical properties of additively manufactured parts. They were able to reduce the time to predict mechanical properties of their composite laminates using this technique. Qi et al. [95] utilised a neural network to predict the tensile strength of 3D printed PLA composites by optimising hyperparameters such as learning rate, number of hidden layers, neurons per layer and dropout rate. Their results demonstrated that a two-layer network with 64 neurons per layer and a learning rate of 0.01 yielded an optimal performance. These studies together underscore a critical role of hyperparameter tuning in enhancing predictive accuracy of machine learning models, particularly for 3D printed composites.

#### 4.1. AI Enhancements and Limitations

AI has enormous potential to significantly enhance existing models in 3D printing using VP by improving various aspects such as data handling, prediction accuracy and real-time data integration. Integrating AI with conventional physical models can optimise the prediction of mechanical properties and provide reliable and robust estimates. However, the use of AI in this field may encounter several limitations worth mentioning to maximise its efficacy.

AI significantly improves data handling by automating data preprocessing, cleaning, and normalising datasets [89]. Specific techniques such as advanced feature engineering and synthetic data generation through generative adversarial networks (GANs) ensure that data inputs are high-quality and consistent [96]. These capabilities enable models to process vast and complex datasets effectively, leading to more accurate and reliable predictions. In addition, with the use of advanced regression models, neural networks and deep learning techniques, AI can capture far more complex relationships within data when compared with conventional models [97]. This capability is anticipated to significantly enhance prediction accuracy [97,98]. Additionally, transfer learning allows models to leverage existing knowledge, thus further improving the performance even with limited datasets [97].

AI models can integrate with real-time monitoring systems, enabling continuous data updates and dynamic adjustments to predictions during the manufacturing process [99]. This real-time data integration ensures that the models remain accurate and responsive to changes. Moreover, adaptive learning capabilities allow AI models to evolve with new data, maintaining high prediction accuracy over time and ensuring consistent performance in dynamic environments [99]. As such, combining AI with conventionally physical models leads to hybrid approaches that leverage the merits of both methods. AI can optimise processing parameters and provide more accurate predictions by quantifying uncertainties in order to achieve robust and reliable estimates of mechanical properties. This integration eventually gives rise to a more comprehensive and precise modelling process.

Despite significant advantages of AI in enhancing existing models, several limitations must be addressed. AI models, particularly machine learning algorithms, require large datasets for training and validation [100]. The variability in epoxy resin formulations and DLP-based printing parameters makes compiling comprehensive datasets quite challenging [43]. Practical solutions include implementing data augmentation techniques to artificially expand datasets and encouraging close collaboration between research institutions, industry and 3D printing communities to share and compile more comprehensive datasets. Conversely, AI models trained on specific datasets may be required to generalise better to unseen conditions or epoxy resin formulations, thus limiting their applicability across different DLP-based printing setups. Specific solutions include employing transfer learning and domain adaptation strategies to enhance model generalisation, as well as establishing robust validation protocols to test models under unseen conditions [100,101]. Another aspect to consider with AI models, especially deep learning networks, is that they are often described as "black boxes" due to their complex internal mechanisms, which hinders a better understanding as to how various factors influence 3D printing outcomes [102]. Practical solutions include utilising explainable AI (XAI) methods to increase model transparency and developing hybrid models combining AI with conventional modelling techniques, thereby resulting in predictive power and interpretability.

DLP-based 3D printing of epoxy resins is a dynamic process with evolving properties during curing processes, in which AI models might require necessary assistance to capture if training data do not adequately represent the entire cycle. Combating this limitation requires integrating time-series analysis and dynamic modelling approaches to capture temporal aspects and incorporating real-time monitoring data from sensors embedded in DLP-based printing setup [103,104].

AI has the potential to revolutionise VP printing by improving data handling, prediction accuracy, real-time integration, as well as hybrid modelling. Current AI techniques, enabling the assistance in predicting mechanical properties of 3D printed resin composites, can be found in Table 1. Addressing the limitations, such as data dependency, interpretability, generalisation and dynamic process modelling through specific strategies, can further enhance the effectiveness of AI technologies. By overcoming these challenges, AI provides robust, accurate and reliable models for predicting mechanical properties in resin composites in AM advanced field.

Table 1. AI techniques used for predicting the mechanical behaviour of 3D printed resin composites.

AI Technique	Description	References			
Improved Data Handling					
Data Preprocessing and Cleaning	AI algorithms automate data preprocessing tasks, ensuring high-quality data inputs for predictive models. They correct outliers, fill missing values and standardise data formats.	[89,105,106]			
Data Augmentation	GANs are used to create realistic synthetic data that mimics the distribution of original data, thereby expanding the training set and improving model robustness. Enhanced Prediction Accuracy	[96,107,108]			
Advanced Regression Models	Advanced regression models like support vector machines (SVM), decision trees and ensemble methods provide accurate predictions by combining multiple algorithms.	[109,110]			
Neural Networks and Deep Learning	Neural networks, including convolutional neural networks (CNNs) and recurrent neural networks (RNNs), capture complex nonlinear relationships in data, thus improving prediction accuracy.	[97,98,111]			
Transfer Learning	Transfer learning pre-trains models on large datasets and fine-tunes them on specific smaller datasets, leveraging existing knowledge to improve model performance.	[112,113]			
Real-Time Monitoring and Feedback	<i>Real-Time Data Integration and Adaptive Learning</i> AI models integrated with real-time monitoring systems continuously update predictions based on live data for the optimisation of 3D printing processes.	[114–116]			
Adaptive Learning Systems	Al systems that continuously learn from new printing results and material properties automatically update predictive models to reflect the latest information and trends.	[99,117]			
Hybrid Modelling Approaches	Integration with Physical Models The combination of AI with conventional physical models creates hybrid models that enhance prediction accuracy and applicability to various materials. Bayesian neural networks (BNNs) can belo quantify uncertainties in predictions	[81,118,119]			
Uncertainty Quantification	providing more robust and reliable estimates of mechanical properties. They facilitate probabilistic predictions with confidence intervals, helping understand the uncertainty and reliability of model outputs.	[120–124]			
Genetic Algorithms	Techniques like genetic algorithms (GAs) and particle swarm optimisation (PSO) optimise filler configurations and 3D printing parameters to improve mechanical properties.	[123–126]			
Clustering Algorithms	Clustering algorithms and principal component analysis (PCA) reveal patterns and key variables in data in order to optimise composite formulations and improve model accuracy.	[127-129]			

#### 4.2. Improved Data Handling

4.2.1. Data Preprocessing and Cleaning

AI algorithms can automate data preprocessing tasks, such as cleaning, normalising, and transforming raw data into usable formats. These algorithms can ensure high-quality data inputs for predictive models. The use of AI-driven tools to identify and correct outliers, fill missing values and standardise data formats, thus enhancing the consistency and reliability of the dataset. For example, Goyle et al. [105] discussed how AI can automate data cleaning and preparation tasks, improving the quality of datasets for machine learning models. It uses machine learning algorithms to highlight methods like missing value imputation, outlier detection and data normalisation [105]. Hosseinzadeh et al. [106] covered

various data cleansing mechanisms and approaches for big data analytics, emphasising the role of AI in improving data quality through automated preprocessing tasks [106]. They also presented an automated preprocessing pipeline that leverages AI to handle data transformation, normalisation and feature engineering, significantly enhancing the efficiency of data preparation for machine learning [106].

AI-driven tools can identify and correct errors, handle missing values, remove duplicates and detect outliers [105,106]. These tools use statistical methods and machine learning algorithms to identify patterns and anomalies in the data, ensuring that the cleaned dataset is accurate and reliable [105,106]. For example, DataAssist employs machine learning techniques to handle various data preprocessing tasks, including detecting and correcting duplicates and inconsistencies [105]. Additionally, AI algorithms can automatically normalise data, ensuring that numerical features are scaled to a common range, such as 0 to 1, or standardised using techniques like Z-score normalisation [105]. This step is crucial for improving the performance of machine learning models because it ensures that all features contribute equally to the model predictions. Specific techniques like min–max scaling and Z-score standardisation are commonly used to prepare data for machine learning tasks [105,106].

AI can assist in feature engineering by creating new features from existing data in order to better represent the underlying problem to machine learning models. This feature engineering includes encoding categorical variables, creating interaction terms and extracting meaningful features using particular techniques like principal component analysis (PCA) or autoencoders [105,106]. Machine learning techniques, such as feature selection and extraction, can identify the most relevant features affecting mechanical properties. These techniques can reduce dimensionality and improve model efficiency. For example, PCA or autoencoders automatically extract key features from complex datasets for model simplification without losing critical information [105,106].

# 4.2.2. Data Augmentation

AI techniques generate synthetic data to augment small datasets for addressing the issue of limited data availability and enhancing model training and validation [96]. GANs are used to create realistic synthetic data that mimics the distribution of original data, thereby expanding the training set and improving model robustness and performance. Ramzan et al. [107] discuss how GANs can generate synthetic datasets that replicate statistical properties of original financial data, in focus of data scarcity and privacy issues, as seen in Figure 6. The synthetic data generated can mimic the distribution of stock prices, trading volumes, and market trends to enhance the robustness and generalisation of machine learning models [107].



Figure 6. GAN architecture [107].

Chakraborty et al. [96] highlight the versatility of GANs in various applications, including data augmentation for video and text generation and medical image synthesis. It discusses the challenges and advancements in GAN training, such as improving stability and performance. Chakraborty et al. [96] also explored using GANs to generate synthetic numerical datasets. It describes the architecture and parameters of GANs used and evaluates the quality of synthetic data in terms of its ability to improve the performance of machine learning models on small and imbalanced datasets [96]. Biswas et al. [108] discussed the use of GANs for augmenting training data in various domains, including medical imaging and fraud detection. It emphasises how GANs can alleviate class imbal-

medical imaging and fraud detection. It emphasises how GANs can alleviate class imbalance by generating synthetic data samples that resemble real data, thus improving model training outcomes [108]. AI techniques, particularly GANs, can generate synthetic data to augment small datasets, addressing the issue of limited data availability. This technique can significantly enhance model training and validation by providing more diverse and comprehensive datasets.

# 4.3. Enhanced Prediction Accuracy

# 4.3.1. Advanced Regression Models

Machine learning algorithms, such as SVM, decision trees, and ensemble methods like random forests and gradient boosting, can offer more accurate predictions than conventional linear models [109]. Implementing ensemble methods to combine multiple predictive models enables to improve the accuracy by reducing the variance and bias of individual models. Such advanced regression models leverage the strengths of multiple algorithms to improve prediction accuracy and robustness. Ensemble methods to combine multiple predictive models are proven to enhance the accuracy with the reduction of variance and bias for individual models [110]. For example, using random forests, which is combined with the predictions of multiple decision trees, can significantly improve model performance, as opposed to using a single decision tree [109]. Liang et al. [130] found that using machine learning techniques successfully predicted thermal conductivity of polymer composites. Such techniques reduced the requirement for substantial amounts of testing and improved the generalisation ability and accuracy of models according to Figure 7. Additionally, Gao et al. [131] also reduced experimentation time through the use of a data-driven process–quality–property (PQP) framework for FFF-based conductive composites.



**Figure 7.** Machine learning technique using a co-artificial neural network (co-ANN) to predict thermal conductivity ability of polymer composites [130].

Gupta et al. [109] compared the performance of various machine learning algorithms, including SVM, decision trees and ensemble methods, which highlight their effectiveness in the provision of accurate predictions. It demonstrates that ensemble methods, such as random forests and gradient boosting, outperform conventional models in various applications. This review also discusses current advancements in ensemble methods, explaining how these techniques are combined with the predictions of multiple models to improve accuracy and robustness. Ardabili et al. [110] explored the applications of SVM and decision trees by demonstrating their capabilities in handling high-dimensional data and complex relationships. Special examples used were the applications for hybrid and ensemble methods that included signal processing and wave height prediction respectively. It also discussed

the advantages of using ensemble methods to combine such algorithms, resulting in more accurate and dependable predictions. By incorporating these AI technologies, researchers can effectively reveal how advanced regression models and ensemble methods enable to improve prediction accuracy and robustness in 3D printed resin composites.

# 4.3.2. Neural Networks and Deep Learning

Neural networks, including deep learning models like convolutional neural networks (CNNs) and recurrent neural networks (RNNs), can capture complex and nonlinear relationships in the data [97,98]. Using CNNs to model spatial relationships in composite materials or RNNs to predict time series data on the aging and degradation of materials leads to more precise predictions [111]. Neural networks are highly effective in capturing complex and nonlinear relationships in data. These models are particularly useful for specific tasks involving spatial and temporal data. CNNs are adept at recognising patterns and spatial hierarchies within data, while RNNs are suitable for sequential data due to their ability to maintain the memory of previous inputs [97,98]. For instance, Babichev et al. [97] emphasised the proficiency of CNNs and RNNs in capturing nonlinear relationships in high-dimensional gene expression data. It is clearly shown how these models can autonomously learn feature representations from raw data for improving classification accuracy and reducing bias incorporation during the process of manual feature extraction.

#### 4.3.3. Transfer Learning

Transfer learning involves pre-training models on large datasets and fine-tuning them on specific and smaller datasets [112]. This approach leverages existing knowledge to improve model performance. It comprises the pre-training of a neural network on a large dataset of mechanical properties for various materials, then fine-tuning it for specific particle-reinforced resin composites, and finally enhancing prediction accuracy with limited data [113]. This approach leverages existing knowledge to improve model performance by transferring information learned from one domain to another. It is particularly useful when limited data are available for a target task [112].

Hosna et al. [112] gave a comprehensive overview of transfer learning, along with detailed discussions regarding various strategies and scenarios where transfer learning can be effectively applied. Figure 8 shows the comparison between conventional machine learning and transfer machine learning. It highlights the benefits of pre-training models on large datasets and fine-tuning them on smaller and task-specific datasets, thereby significantly improving model performance. Meanwhile, Ye [132] discussed different pre-training strategies and their effectiveness in various applications. It emphasised the importance of selecting appropriate sources and target domains to avoid negative transfer and improve learning performance. This work provides good examples of successful transfer learning implementations, such as using pre-trained models in computer vision tasks.

Furthermore, Rafiq and Albert [113] explored the mechanics of transfer learning, including how pre-trained models can be adapted to new tasks with smaller datasets. It discussed the concept of domain adaptation and the techniques used for fine-tuning models for specific applications, thereby enhancing their accuracy and efficiency. Equally important is the study carried out by Wang and Chen [133], which detailed the process of pre-training models on large-scale datasets to capture general features and subsequently fine-tune them for specific tasks. This research discussed the benefits of this approach in improving model generalisation and performance, particularly in scenarios with limited data availability for a target task. Transfer learning can be used to enhance predictive modelling in 3D printed resin composites. The use of pre-trained models and their fine-tuning for specific materials offers potential benefits of this approach in improving prediction accuracy and model robustness.

24 of 40



# Learning Methods in Traditional and Transfer Machine Learning

Figure 8. Comparison between conventional machine learning and transfer machine learning [112].

4.4. Real-Time Data Integration and Adaptive Learning

4.4.1. Real-Time Monitoring and Feedback

AI models can be integrated with real-time monitoring systems to continuously update predictions based on live data from the manufacturing process [114,115]. Sensors can collect real-time data on printing parameters and mechanical properties, feeding this data into AI models to dynamically adjust predictions and optimise printing processes during the production [116]. This integration allows for dynamic adjustment and optimisation of the printing process on the fly, enhancing efficiency and accuracy. Keleko et al. [114] mentioned using AI for predictive maintenance in Industry 4.0 in focus of the importance of real-time data integration for improving productivity and reducing downtime. The study highlighted how AI-driven real-time monitoring systems enabled to provide continuous feedback, thus allowing immediate adjustment and optimisation.

Furthermore, Cakir et al. [116] detailed the implementation of real-time big data solutions in manufacturing, including AI for monitoring and analysing sensor data. The study highlighted direct benefits of real-time data processing for making immediate decisions and optimising production processes. By using sensors to collect and process live data and dynamic adjustment enabled by AI models, efficiency and accuracy tend to be improved for 3D printed resin composites.

# 4.4.2. Adaptive Learning Systems

Implementing adaptive learning algorithms allows models to evolve and improve as new data become available towards high prediction accuracy over time [99]. The application of adaptive learning algorithms allows the models to evolve and improve upon the availability of new data to achieve high prediction accuracy. These systems continuously learn from new inputs, such as printing results and material properties, updating the predictive model to reflect the latest information and trends [117]. For example, Ezzaim et al. [99] reviewed state-of-the-art AI-based adaptive learning, focusing on how these systems can dynamically adjust to new data to enhance learning outcomes. It stressed the importance of continuous learning and model updating in maintaining high prediction accuracy. They also systematically mapped AI-enabled adaptive learning systems, discussing how they leveraged continuous data input to refine and improve their predictive capabilities. The study showcased various adaptive learning applications in education and industry, highlighting direct benefits of dynamic model adjustments. The use of adaptive algorithms to learn from real-time data and update models accordingly will lead to an enormous potential of these AI systems to enhance the performance and reliability of 3D printed resin composites.

#### 4.5. Integration with Physical Models

# 4.5.1. Hybrid Modelling Approaches

The combination of AI models and conventional physical models, such as Halpin–Tsai model, can create hybrid models that leverage reciprocal strengths [81]. This means using AI to optimise the related parameters in Halpin–Tsai model based on empirical data, thus enhancing its accuracy and applicability to a wider range of materials and conditions [81,118]. Hassanzadeh-Aghdam and Jamali [81] presented a modified Halpin–Tsai model for characterising mechanical properties of CNT-reinforced polymer nanocomposites. It highlights the integration of AI techniques to modify model parameters, which improves the accuracy of predictions relative to conventional models. In contrast, Alfonso et al. [118] used FEA combined with modified Halpin–Tsai models to estimate elastic properties of particulate-reinforced composites. This hybrid approach enhances its ability to predict material behaviour under various conditions.

Additionally, Zhu et al. [119] explored the use of hybrid models combining conventional micromechanical approaches with AI-based optimisation techniques. This method allows for more precise modification of model parameters, leading to better accordance with experimental results and improved predictive performance. Integrating AI techniques with Halpin–Tsai model shows promising potential to improving the accuracy of mechanical property predictions for 3D printed resin composites reinforced with particles. By leveraging machine learning algorithms to optimise *k*-parameter and other empirical factors in Halpin–Tsai model, researchers can better account for complex interactions between resin matrices, reinforcing particles and unique microstructures created by DLP process. This hybrid approach allows for more precise estimations of elastic modulus and strength across a wider range of particle types, sizes, and volume fractions, as typically used in 3D printed resin composites.

# 4.5.2. Uncertainty Quantification

AI can help quantify uncertainties in predictions, providing more robust and reliable estimates of mechanical properties [120] and implementing Bayesian neural networks (BNNs) to yield probabilistic predictions with confidence intervals, which helps to understand uncertainty and reliability of model outputs [120]. BNNs incorporate uncertainty by treating model weights as distributions rather than fixed values, allowing the model to provide predictions with a measure of confidence [120]. Mosser and Naeini [120] discussed the application of BNNs for uncertainty quantification in data-driven models. It highlights the importance of incorporating uncertainty estimates to enhance robustness and reliability of predictions, particularly in safety-critical applications. They explored using Bayesian convolutional neural networks (BCNNs) to provide calibrated probabilistic predictions. It demonstrates how BCNNs can quantify epistemic (model) and aleatoric (data) uncertainties, thereby improving a good understanding of model predictions in geophysical applications. BNNs offer a significant advantage in predicting mechanical properties of 3D printed resin composites by providing probabilistic predictions with confidence intervals [120]. This capability is particularly valuable when dealing with inherent variability in DLP process, such as some variations in resin curing, particle dispersion and interfacial adhesion. BNNs enable engineers to make more informed decisions about material formulations and printing parameters by quantifying the uncertainty in predicting elastic modulus, tensile strength and fracture toughness. For instance, when optimising the volume fraction of reinforcing particles in a DLP-based composite, confidence intervals provided by BNNs can help to identify the range of particle concentrations in order to achieve desired mechanical properties with the consideration of process-induced uncertainties.

# 4.6. Optimisation Techniques

#### 4.6.1. Genetic Algorithms (GAs)

Genetic algorithms (GAs) can explore a vast search space of possible filler configurations and processing parameters to identify optimal solutions that might not be evident

through conventional methods [134]. GAs can be employed to optimise the selection and distribution of fillers within resin matrices to improve mechanical properties of composites. The exploration process involves crossover, mutation and selection operations, which allow GAs to navigate complex optimisation landscapes and then find high-quality solutions [134,135]. These algorithms simulate the process of natural selection by generating, evaluating and evolving potential solutions iteratively until an optimal solution is found [125]. To demonstrate this, Kumpati et al. [125] revealed the use of multi-objective genetic algorithms to optimise the stacking sequence of composite laminates, as illustrated in Figure 9. The genetic algorithm effectively handled multiple design constraints and objectives, indicating its ability to find optimal configurations for improved mechanical properties. Likewise, Bommegowda et al. [134] highlighted various methods to enhance mechanical properties of polymer composites, including optimising filler distribution using advanced algorithms like GAs. It emphasises the effectiveness of GAs in exploring and identifying the best filler configurations to achieve desired property enhancements. The ability of GAs to explore complex search spaces and find optimal solutions will promote their potential benefits in improving mechanical properties through innovative computational techniques.



Figure 9. A block diagram of a multi-objective evolutionary strategy [125].

Genetic algorithms (GAs) offer several advantages for optimising filler configurations in 3D printed composites, particularly due to their robustness in handling discrete variables and the ability to explore complex solution space through specific operations like crossover and mutation [136]. Such characteristics make GAs well-suited for typical problems with numerous constraints and interacting variables, such as those encountered in composite material design [125]. However, as opposed to PSO, GAs may require more computational resources and iterations for convergence with potentially less efficiency [137,138]. PSO is generally simpler to implement, with fewer parameters to tune, and often converges faster for continuous variable problems. The choice between GAs and PSO ultimately depends on a specific nature of optimisation problems encountered, including the one whether it involves predominantly discrete or continuous variables [138].

#### 4.6.2. Particle Swarm Optimisation (PSO)

Particle swarm optimisation (PSO) can be used to optimise printing parameters (e.g., layer height, print speed, curing time) to enhance mechanical properties of 3D printed

composites [124]. PSO can efficiently navigate complex optimisation landscapes by providing solutions that balance competing objectives such as strength, durability and print time [126]. Ali and Hussein [124] explored the use of PSO to optimise mechanical properties of materials. By integrating PSO with CNNs, the research demonstrates significant improvements in material performance, highlighting the ability of PSO to explore and optimise complex parameter spaces efficiently. Additionally, Murat et al. [139] discussed how PSO was used to optimise processing parameters of selective laser melting (SLM). The study has shown that PSO can effectively identify optimal settings that enhance mechanical properties while balancing production speed and material usage.

Furthermore, Seyedzavvar [126] combined artificial neural networks (ANNs) with PSO to optimise material composition and processing parameters in 3D printing. The hybrid approach demonstrated improved mechanical properties of printed samples, indicating the effectiveness of PSO in multi-objective optimisation scenarios. Finally, Shirmohammadi et al. [140] demonstrated using PSO in conjunction with neural networks to optimise 3D printing parameters, achieving significant surface roughness reductions along with improved print quality. This study reveals practical applicability of PSO in promoting the precision and quality of 3D printed parts. PSO possesses significant potential to optimising mechanical properties of 3D printed resin composites by simultaneously balancing multiple objectives such as tensile strength, elastic modulus and fracture toughness [126]. When applied to DLP process, PSO can efficiently explore the complex landscape of printing parameters, including layer thickness, curing time and light intensity, along with material formulation variables like filler type, size and concentration. This capability allows for fine-tuning processing parameters and material composition to achieve optimal mechanical performance in 3D printed resin composites. This potentially leads to very competitively designed parts with enhanced strength-to-weight ratios, higher impact resistance and well-tailored flexibility for specific applications.

#### 4.7. Data Mining and Pattern Recognition

# 4.7.1. Clustering Algorithms

Using clustering algorithms (e.g., k-means, hierarchical clustering) can help identify patterns and group similar filler-resin combinations based on their mechanical performance [127,128]. Clustering can reveal underlying trends and relationships in the data that are not apparent through conventional analysis, leading to great insights into effective composite formulations [127,141]. By grouping similar data points, clustering algorithms help better understand the distribution and impact of various fillers within resin matrices, which presents a clearer picture of how different combinations affect resulting mechanical properties [141]. For instance, Chaudhry et al. [127] covered clustering algorithms in data mining to achieve data segmentation into meaningful groups. Figure 10 shows the categorisation of data mining techniques. It emphasises how clustering can uncover valuable information by grouping data points based on statistical similarities, which is crucial to identify effective composite formulations in 3D printed resins. Rodriguez et al. [128] also provided a comparative analysis of various clustering algorithms, including k-means and hierarchical clustering. It discusses the performance of these algorithms in different contexts and their ability to identify patterns and trends in complex datasets, such as those used in material science for the optimisation of composite formulations. The ability of clustering to reveal hidden patterns and optimise composite formulations highlights practical benefits of using such techniques in analysing 3D printed resin composites.





# 4.7.2. Principal Component Analysis (PCA)

The most significant variables influencing mechanical properties can be identified by applying principal component analysis (PCA) to reduce data dimensionality [129]. PCA enables to simplify complex datasets by projecting high-dimensional data onto a lower-dimensional space, which captures the maximum variance in the data [142]. This process enhances interpretability and accuracy of predictive models because it helps isolate the most impactful variables and reduce noise from less significant ones. To demonstrate this, Migenda et al. [129] explored the application of PCA for reducing data dimensionality in real-time settings. It demonstrates how PCA can transform high-dimensional data into a set of orthogonal components to preserve the variance and simplify the data structure. This approach benefits specific applications where continuous data streams must be analysed efficiently.

Moreover, Bisong [142] discussed the fundamentals of PCA, including its ability to project data onto orthogonal axes and reduce the number of dimensions. It highlights how PCA is used to identify the most significant variables in datasets, which is crucial for improving the accuracy and interpretability of predictive models in various fields like material science. A comprehensive overview of PCA is also considered as an effective method for reducing the dimensionality of large datasets. It explains how PCA can simplify the data by capturing essential features that account for the most variance, which makes it easier to analyse and interpret complex datasets effectively. The ability of PCA to reduce dimensionality and identify key variables underscores its importance in improving interpretability and accuracy of predictive models.

# 4.8. Bayesian Inference and Probabilistic Models

# 4.8.1. Bayesian Networks

Bayesian networks can model probabilistic relationships between variables with the incorporation of uncertainty and variability in the predictions [122]. They are graphical models representing variables and their conditional dependencies through directed acyclic graphs, which are particularly effective for handling uncertainty [122]. Bayesian networks offer a robust framework for handling uncertainty by integrating prior knowledge and observed data to provide more reliable predictions [121]. This integration allows for a comprehensive understanding of probabilistic relationships among variables, making Bayesian networks a powerful tool for decision-making under uncertainty [122]. Tosun et al. [122] emphasised the robustness of Bayesian networks in integrating prior knowledge with observed data to improve prediction accuracy and reliability. In comparison, Du and Swamy [121] illustrated how Bayesian networks could efficiently manage uncertainty by representing conditional dependencies among variables. Furthermore, Su et al. [143] explored using Bayesian networks in genetic research to uncover special relationships be-

tween genes, environmental factors and diseases. It demonstrates how Bayesian networks can decompose complex systems into smaller and manageable components for detailed probabilistic analysis and a better understanding of underlying relationships.

In a similar manner, Yamawaki et al. [144] enabled the prediction of the decomposition degree using Bayesian optimisation for biobased polymers. This model shows a good correlation with experimental results. Integrating prior knowledge with observed data underscores the reliability and robustness of Bayesian networks in enhancing predictive models for 3D printed resin composites. Liu et al. [44] used statistical learning and optimisation within a nonparametric Bayesian framework to discover required processing parameters in nanocomposite design and part fabrication. Their framework was able to identify optimal parameters within five iterations. It was identified that this process could be used for other nanocomposites. In addition, Albuquerque et al. [145] created novel biobased epoxy resin systems using Bayesian optimisation and active learning techniques. Their study used epoxy resins as the matrices for fibre-reinforced composites with a high  $T_g$ . They were then able to create epoxy-based resins also with a higher  $T_g$ , depending on only five samples via Bayesian optimisation shown in Figure 11.



Figure 11. The workflow for Bayesian optimisation reported by Albuquerque et al. [145].

#### 4.8.2. Gaussian Processes

Gaussian processes (GPs) can be implemented for non-linear regression and uncertainty quantification in predicting mechanical properties [146]. GPs provide a flexible and probabilistic approach to regression, effectively modelling complex relationships within the data [146]. They capture uncertainty in predictions by defining a distribution over functions for data fitting, which offers great insights into confidence levels of model outputs [146]. This capability makes GPs particularly suitable for applications requiring a crucial understanding of the reliability of predictions. Kobayashi et al. [146] explored how Gaussian processes could be used for non-linear regression and uncertainty quantification. It highlights the advantages of GPs in expressing uncertainty for predictions and their effectiveness in various scientific fields. This study illustrates the application of Gaussian processes in digital twin models for accident-tolerant fuel, revealing the flexibility of GPs in handling uncertainty and providing reliable predictions in engineering contexts. Marrivada et al. [147] used Gaussian Process Regression (GPR) with machine learning techniques to successfully build predictive models for their research involving composites with graphene nanoplatelets. Their model could estimate stress-strain curves from experimental results with good correlation. In addition, Park et al. [148] also used GPR to model platelet arrays. Their findings indicate that GPRs can use a limited number of computational simulations or experiments for material optimisation problems. GPs offer a significant advantage in predicting mechanical properties of 3D printed resin composites by capturing and quantifying uncertainties associated with material variability and processing parameters [146]. This capability is particularly valuable for DLP-based composites, where factors such as resin curing kinetics, particle dispersion and layer adhesion can induce significant variability in mechanical performance. By providing probabilistic predictions of elastic modulus, tensile strength and fracture toughness, GPs enable engineers to assess the reliability of their predictions and identify potential sources of variability in 3D printing processes.

# 5. Comparative Analysis of Fillers

A detailed comparative analysis of different fillers demonstrates that their combined use can significantly enhance mechanical properties. For instance, ceramic fillers are known for their excellent hardness and thermal stability, while rubber fillers contribute to the improvements in flexibility and impact resistance [149,150]. On the other hand, recycled resin fillers offer a sustainable option by reusing material waste, which can also enhance specific mechanical properties, depending on material characteristics of original resins [151]. This integrated approach allows for identifying optimal filler combinations that can achieve desired mechanical outcomes more effectively instead of just relying on a single type of fillers. The combination of ceramic fillers and rubber fillers results in a combined hard and flexible material, leading to a balanced performance profile suitable for high-stress applications [149,150]. This synergistic approach has a significant impact in various specialised fields. In biomedical devices, for instance, the combination of fillers can be tailored to achieve specific properties such as biocompatibility, flexibility and strength, which are critical for implants and prosthetics [152]. High-performance engineering components, such as those used in aerospace and automotive industries, can benefit from fillers with better thermal stability, higher strength and durability to improve overall performance and life expectancy.

The synergistic effects of combining multiple fillers can be attributed to several key mechanisms in terms of size effects, interfacial interactions and the formation of interconnected networks within composite materials, as seen in Table 2:

Synergistic Effects	Role	Evidence
Complimentary size effects	<ul> <li>Smaller particles can fill the gaps between larger ones, leading to a more efficient packing structure</li> <li>Enhanced packing</li> <li>Improves stress transfer</li> <li>Reduces void content</li> </ul>	<ul> <li>Use of nanoparticles [152,153]</li> <li>Improvement of mechanical properties [154]</li> <li>Scattering effects of fillers to alter cure depth [155]</li> </ul>
Interfacial interactions	• Between filler and polymer matrix	<ul> <li>Improving dispersion and strengthening the matrix-filler interface [156].</li> <li>Enhancing crosslinking and reducing inhomogeneity in printed layers [157].</li> <li>Formation of interfaces before or after curing [158].</li> <li>Surface chemistry and wettability of fillers [159].</li> <li>Interfacial interactions to improve mechanical properties [160].</li> <li>Rheological properties [161].</li> <li>Rheological percolation occurring at different filler concentrations [162]</li> </ul>
Interconnected networks	• Fillers with different aspect ratios, can lead to enhanced mechanical reinforcement, improved electrical or thermal conductivity and increased resistance to crack propagation	<ul> <li>Significant enhancement of properties [163–165]</li> <li>Fillers with different aspect ratios [166]</li> <li>Percolation thresholds and conductivity with filler network alignment [167]</li> </ul>

Table 2. Summary of synergistic effects of combining multiple fillers.

From a cost-performance perspective, synergistic effects can allow for using low-cost fillers combined with more expensive counterparts in order to achieve similar or better properties when compared with single high-performance fillers [168]. This combination opens up enormous opportunities for cost reduction in high-performance composites and improved material sustainability through biobased or recycled fillers. More importantly, leveraging synergistic effects enables the manufacture of multifunctional composites, where multiple enhanced functionalities, such as mechanical reinforcement combined with self-healing capabilities or improved flame retardancy alongside enhanced electrical conductivity, can be achieved simultaneously for global optimisation of material properties.

A holistic analysis provides a framework for systematically exploring new filler combinations and their effects on mechanical properties. This analysis can develop advanced composite materials with customised properties for specific applications. By understanding the interactions between different fillers and resin matrices, researchers can optimise material formulations in order to meet stringent requirements of various industries.

# 6. Theoretical Predictions for Practical Applications

Theoretical models presented offer strong indication of their practical applications. They provide a holistic framework that can be used to guide experimental investigation and practical use in various industries. By predicting mechanical properties of resin composites with high accuracy, these models serve as an essential tool for practical applications. The insights gained from these models can help understand the underlying mechanisms of material behaviour, thereby demonstrating the development of more effective 3D printing processes.

Theoretical predictions outlined in this study offer a roadmap for optimising 3D printing processes and material selections to achieve desired mechanical properties. By providing a detailed understanding of how different variables affect mechanical properties of resin composites, such models enable researchers and engineers to make reasonable decisions about processing parameters and material formulations. For instance, the detailed knowledge regarding how specific fillers interact with resin matrices allows for precise tuning of material formulations to enhance strength, flexibility or other desired properties. Specific parameters such as layer height, print speed and curing methods can be adjusted based on the insights offered by the models to improve both quality and performance of 3D printed parts. This approach reduces the demand for extensive "trial and errors" methods, saving time and resources while increasing the efficiency of development processes. A good alignment of theoretical predictions with practical applications can significantly benefit industries that rely on high-performance composite materials. Such models can help select optimal composite formulations that meet specific mechanical requirements in aerospace and automotive sectors for critical material performance. Similarly, in biomedical applications where biocompatibility and mechanical integrity are paramount, the models are able to guide the development of materials to warrant safety and efficacy.

The choice between theoretical micromechanical models and AI techniques depends on specific requirements of end users. For rapid and physically interpretable predictions, micromechanical models might be preferred for mechanical property prediction in a timely manner. For more accurate predictions across a wide range of materials and parameters in complex situations, AI techniques could be a better option. A hybrid approach combining both methods might offer the best balance for many applications in DLP-based resin composites. A comparison of micromechanical models and AI techniques can be found in Table 3.

	Micromechanical Models	AI Techniques	
Accuracy	• Accurate for specific scenarios, but often with calibration against experimental data	• Higher accuracy by capturing complex and non-linear relationships, as well as patterns in large datasets	
Complexity	Generally less complex based on established composite theory	• More complex in terms of implementation and interpretation	
Advantages	<ul> <li>Well-established and understood in the field</li> <li>Less computational power</li> <li>Clear physical insights into material behaviour</li> </ul>	<ul> <li>Handling complex and non-linear relationships</li> <li>Potentially more accurate for diverse material compositions and printing parameters</li> <li>Ability to improve predictions with more data</li> </ul>	
Disadvantages	<ul> <li>Required calibration for specific materials</li> <li>Unable to capture all complexities of 3D printed composites</li> <li>Limited in predicting properties beyond their underlying assumptions</li> </ul>	<ul> <li>Required large datasets for training</li> <li>Use of "black box" models with less physical insight</li> <li>Unable to generalise well outside their training data range</li> </ul>	
Context for end user requirements	<ul> <li>Preferred use of AI for more accurate predictions across a wide range of materials and parameters</li> <li>Easier implementation of micromechanical models for end users to understand and apply</li> <li>More AI adaptability to different material compositions and printing parameters</li> <li>Faster predictions once calibrated for micromechanical models</li> <li>Clearer physical insights based on micromechanical models for valuable for material design</li> </ul>		

**Table 3.** A comparison of micromechanical models and AI techniques for predicting mechanical properties of DLP-based resin composites.

# 7. Summary

This study has given significant theoretical insights into the enhancement of predictive models for mechanical properties of 3D printed resin composites. The integration of micromechanical models and AI techniques has been shown to offer a robust framework for accurately predicting mechanical properties. These theoretical findings lay out a solid foundation for optimising 3D printing processes and material formulations, bridging the gap between theory and practical applications. By combining conventional mathematical models with modern AI capabilities, the study reveals a novel approach to material modelling that significantly improves prediction accuracy with a better understanding of essential filler–matrix interaction.

The enhanced predictive models can guide the optimisation of 3D printing processes, improving material performance and efficiency. For instance, the insights gained from the comparative analysis of fillers provide optimal selection and a combination of materials in aerospace, automotive and biomedical industries, in which high-precision and highperformance materials are critical. Such applications demonstrate immediate practical use based on the review in this study so that a roadmap can be created for future experimental work and industrial applications.

Halpin–Tsai model is deemed a fundamental theoretical modelling tool in predicting mechanical properties of composite materials. However, specific assumptions about filler properties and distribution often limit its conventional applications. AI can significantly enhance this model by optimising filler characteristics and their distribution within resin matrices. With the aid of machine learning algorithms and real-time data analytics, AI can dynamically adjust the parameters of Halpin–Tsai model to reflect actual conditions during 3D printing processes. This optimisation results in a more accurate prediction of mechanical properties of composite materials, along with less requirement for extensive empirical testing and rapidly increasing development of new composite material formulations.

The effects of 3D printing parameters, such as layer height, print speed and curing methods, are critical determinants of mechanical properties of 3D printed resins. Layer

height influences the resolution and surface finish of 3D printed parts, with thinner layers typically resulting in better mechanical properties due to enhanced interlayer bonding. Print speed affects exposure time and the degree of polymerisation, with optimal speeds balancing both production efficiency and material performance. Curing methods, including light and thermal sources, are crucial in achieving the desired degree of polymerisation and crosslinking density. AI models can continuously integrate real-time data from these printing parameters, enabling dynamic adjustments to optimise printing processes and improve the consistency and quality of ultimate 3D printed parts.

Integrating AI into modelling and predicting mechanical properties of 3D printed resin composites significant advancement in AM technologies. Researchers can achieve more accurate and reliable predictions by addressing the limitations of conventional models and leveraging advanced AI techniques. This discussion underscores the potential of AI to revolutionise material science, which paves the way for innovative applications in various high-performance fields. The continued exploration and validation of AI-enhanced models and new materials will further drive the evolution of 3D printing technologies, contributing to developing superior composite materials with well-tailored properties for specific applications.

This study has provided valuable theoretical insights and practical recommendations for enhancing mechanical properties of 3D printed resin composites. A combination of both conventional and modern techniques, such as classical composite theory and AI, offers a novel approach to material modelling with a promising AM prospect. Future studies can build upon these findings by addressing identified research gaps and focusing on both theoretical refinement and practical applications to achieve even greater advancements in AM field.

Future research should focus on several key areas to further enhance the integration of AI in 3D printing resin composites. Firstly, there is a high demand for extensive experimental validation of AI-enhanced models in order to warrant their accuracy and reliability in real-world applications. Collaborative efforts between academic institutions and industry can facilitate the sharing of comprehensive datasets, improving the robustness and generalisability of predictive models. Secondly, exploring new filler materials, including biocomposites and nanofillers, may provide great insights into novel applications and also improve environmental sustainability of 3D printing processes. Additionally, developing hybrid models that combine AI with conventional physical models offers a more comprehensive understanding of filler–matrix interaction, thus leading to better optimisation of material properties.

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