

C³M-OMMT Twin: A Causal Process–Structure–Property Digital Twin for Morphology-Aware Mechanical Optimization of OMMT-Modified PLA in Fused-Filament Fabrications

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Research Article

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Posted Date: October 22nd, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-10938883/v1>

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Additional Declarations: No competing interests reported.

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Abstract:

The rising need for mechanically reliable and dimensionally stable biodegradable parts made using fused filament fabrication has led to an increased **interest** in developing organo modified montmorillonite (OMMT) reinforced Polylactic Acid (PLA), however recent research have been primarily focused on how changes to the percentage of fillers used in combination with changes to printing parameters affect the overall physical properties of PLA/OMMT while excluding important relationships such as; the degree of clay exfoliation, melt flow behavior, heat-induced bonding between layers of polymer, topological structure of voids formed during processing, and local fracture sites. In response to these limitations, this study will present C³M-OMMT Twin, a Digital-Twin pipeline that addresses all three critical aspects of OMMT/PLA additive manufacturing including cause/effect relationships of composition and processing conditions, crystallography, and morphologies. ExfoRheo-MAP uses data from X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), transmission electron microscopy (TEM), and dynamic mechanical analysis (DMA) to generate a dispersion-intercalation-rheology state vector representing degree of clay exfoliation or aggregations. This physically based representation allows researchers to directly assess and compare the degree of clay dispersion or aggregation across different samples. ThermoBond-Sense will use both the thermal history generated through reconstruction of layer-by-layer heating-cooling cycles and the inter-road healing generated from varied nozzle temperatures, print speeds, layer heights, and raster angles to predict the formation of bonds between adjacent roadways. The goal is to develop a predictive model for determining the optimal levels of each variable necessary for creating materials with consistent bonding characteristics throughout their entire thickness. MorphoFrac-3D will integrate information collected via Scanning Electron Microscope (SEM), micro-computed tomography (micro-CT), and strain field analysis to create a defect-clay-interface graphs. Additionally, it includes a new index called the Clay Void Interface Fracture Susceptibility Index to enable researchers to assess susceptibility to localized failure at specific locations within the samples. CauPSP-Net will couple the graph produced by MorphoFrac-3D with physics-informed causal learning to differentiate between direct and morphology-mediated effects on tensile, flexural, and impact performance of OMMT/PLA composites. ConBayes-Pareto will identify uncertainty-calibrated optimums for material-process combinations. CounterTwinV will validate the predictions made by C³M-OMMT Twin experimentally. It is anticipated that the optimized region developed using this pipeline will be able to increase tensile strength by up to 59-65 MPa, modulus by up to 3.5 – 4.0 GPa, and flexural strength by up to 88-96 MPa while simultaneously decreasing the void fraction created during processing by up to 35 – 55% as compared to baseline values in practical scenarios. The development of this sequential architecture will provide researchers with a means of improving prediction accuracy, reduce reliance on trial-and-error experimentation, expose potential failure mechanisms, and define a manufacturing window for producing high-quality, reproducible, and sustainable composite components.

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1. Introduction

Polylactic Acid (PLA), due to its renewable source, low temperature processing, good dimensional stability, and compatibility with extrusion based Additive Manufacturing (AM), has become one of the most studied biodegradable thermoplastic polymers used in Fused Filament Fabrication (FFF). However, it still suffers from issues including; brittle failure, moderate impact resistance, poor interlayer adhesion, and defects that are sensitive to fractures and thermal gradients in parts. In order to improve upon some of the aforementioned shortcomings, the addition of Organically Modified Montmorillonite (OMMT) clay to PLA can potentially increase the modulus of the polymer, alter the crystallization characteristics, enhance thermal properties, and improve shear stress transfer across layers within printed PLA structures. The response to applied stresses is highly non-linear due to factors such as the level of reinforcement achieved during printing, which is influenced by variables such as the amount of OMMT added to the polymer matrix, the degree of exfoliation and/or intercalation of individual clay platelets, whether or not agglomerates form during melt processing, the melting point viscosity of the polymeric matrix, the thermal history

experienced during the build process, and the pore structure formed at the interfaces between adjacent layers.

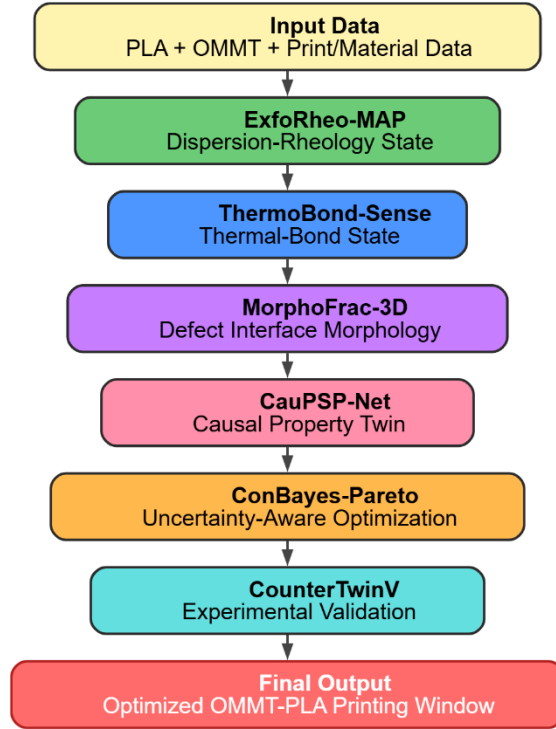


Figure 1. Dataflow of the proposed analytical process

As a result, most studies have evaluated OMMT modified PLA samples through single measurement techniques (e.g., tensile testing, flexural testing, thermal analysis, rheological tests, microscopy etc.), whereas optimization efforts typically employ empirical models (statistical response surface methodology) and/or machine learning algorithms (parameter-to-property mapping) to determine optimal printing parameters. Although this type of approach provides insight into how variations in the state of materials influence their local microstructural evolution and subsequent macroscopic deformation mechanisms; they do little to describe how structural changes caused by layer-bonding and morphological development give rise to localized plastic strain concentrations that ultimately lead to failure. Therefore, even after determining "optimal" printing parameters for specific material states and processes, the ability to extrapolate those results across other states and processes is severely limited.

To address these deficiencies, this research as per figure 1, presents the C³M-OMMT Twin, a novel causally-coupled process–structure–property framework that utilizes the following five modules: ExfoRheo-MAP (nanoclay dispersion & rheology), ThermoBond-Sense (thermal bonding), MorphoFrac-3D (defect morphology), CauPSP-Net (causal mechanical response), ConBayes-Pareto (uncertainty aware multi-objective optimization), and CounterTwin-V (experimental validation). These modules are linked together to create a hierarchical structure where each module builds upon previous ones. Specifically, the ExfoRheo-MAP module describes how nanoclay dispersion affects melt rheology. The ThermoBond-Sense module explains how differences in melt rheology affect thermal bonding. Next, MorphoFrac-3D develops a 3-D model describing how thermal bonding influences defect morphology. Then, CauPSP-Net uses the outputs from the previous modules to explain how defect morphology contributes to mechanical response. Finally, ConBayes-Pareto generates uncertainty aware multi-objective optimization solutions for desired combinations of mechanical performance and reduced void and agglomeration-induced fracture susceptibility. Lastly, CounterTwin-V validates both experimentally and computationally the effects of uncertainties associated with printing conditions on predicted responses.

2. Review of Existing Models used for Analysis

Starting with the early work that involved modifying materials to improve their additive manufacturing (AM) printability and mechanical performance, recent research has progressively moved toward more complete, multi-scale analyses of the relationships among AM processing parameters, material composition, morphology, and final part properties. Specifically, Lin

et al. [1] demonstrated that addition of nano-silica to 3D-printed cementitious systems significantly improved both their printability and ultimate compressive strength. Gupta et al. [2] similarly employed cenospheres to modify composite systems produced via fused deposition modeling (FDM), while Hadi et al. [3] investigated the effect of annealing on the surface and bulk properties of PETG reinforced with organically modified montmorillonite clay (OMMT). In other investigations, Bhayana et al. [4] reported on their findings regarding the use of wood as a filler in biodegradable PLA composites and provided some general guidelines for optimizing the wood content of such composites. Similarly, Kumar et al. [5] have found that carbon nanofibres can be used to significantly enhance the mechanical properties of FDM-produced PLA parts. Bharat et al. [6] also reported that reinforcing FDM-produced PLA with *Lawsonia inermis* resulted in significant improvements in its impact resistance and mechanical properties.

Furthermore, Valizadeh and Aslani [7] demonstrated that the incorporation of nanoclays into PETG can result in improved piezoresistive behaviour. However, Karimi et al. [8] established that environmental temperature is a critical variable influencing fracture in FDM-produced PLA. Finck et al. [9] conducted comparative analyses of Fused Deposition Modeling (FDM) fabricated parts made using Digital Light Processing (DLP) and Liquid Crystal Display (LCD) processes. Finally, Ahlawat et al. [10] conducted investigations to determine whether the mechanical properties of FDM produced graphene-PLA composites could be effectively optimised using Multi Objective Genetic Algorithm – Artificial Neural Network (MOGA-ANN) process. In related investigations, Aihemaiti et al. [11] determined the potential benefits of employing ultrasound-assisted additive manufacturing to produce hybrid HA-PLA parts. Kumar Patro et al. [12] also investigated the structural integrity of FDM-produced PLA/ABS sandwich panels. Additionally, Senaysoy et al. [13] demonstrated that biodegradation results in deviations from expected mechanical behaviour in FDM-produced PLA scaffolds. Moreover, Sahin et al. [14] performed an investigation into the weldability of multi-material parts produced via FDM using different types of PLAs. Singh and Francis [15] developed $Mg(OH)_2$ -modified PLA fixation plates for bone repair applications. Likewise, Lei et al. [16] investigated the mesostructures of FDM-produced PLA-GNP composites. Also, Thakur et al. [17] utilised Response Surface Optimisation to investigate how the mechanical properties of FDM-produced PLA composites can be improved. Murugan and Kattimani [18] characterised the surface behaviour of PLA-BTO composite films prepared by solution casting method. Rodríguez-Reyna et al. [19] studied the heat-treatment conditions necessary to achieve optimal mechanical and thermal properties of PLA parts fabricated by extrusion or injection moulding. González González et al. [20] investigated the thermal and morphological changes associated with the degradation of PLA scaffold samples exposed to high temperatures over long durations.

Storch et al. [21] investigated the potential use of spherosilicate particles as reinforcement agents for improving the surface properties of FDM-produced PLA parts. Benali and Le Duigou [22] carried out a study on the effects of thermo-mechanical fatigue on the colouration and crystallinity degree of PETG, which exhibited excellent photochromism and electrochromic abilities under UV light illumination scenarios. Guigot et al. [23] identified that when subjected to long-term exposure to humid environments, the delamination occurring at inter-layer interfaces within layered 3D-printed structures can lead to loss of mechanical integrity in process. Saravanamuthukumar et al. [24] studied the mechanical and thermal behaviours of PLA-Almond Shell Composites. Alphonse et al. [25] also assessed the microstructure and mechanical responses of β -TCP/PLA composites produced using melt-extrusion based 3D printing technology. Zeynivandnejad et al. [26] investigated the effects of degradation on the physical behaviour of hybrid PLA/Mg alloy materials. Birosz et al. [27] investigated the effects of thermal annealing on the mechanical properties and morphology of amorphous polystyrene (PS) materials. Rahman et al. [28] designed scaffold geometries capable of providing mechanical support while being degraded over temporal instance sets. Guessasma and Belhabib [29] demonstrated that in order to understand fully the complex mechanisms involved in 3D printing polymer-based composite materials with good thermal insulation capabilities, it was essential to examine them simultaneously from three complementary viewpoints: thermal, microstructural and mechanical. Furthermore, Riyaz Ahmed and Mugendiran [30] studied how various process parameters affect the mechanical properties of liquid-crystal-display (LCD)-based additive-manufactured PLA parts. Recent investigations increasingly demonstrate a pressing need for a causal model that integrates multiple aspects instead of treating each separately. For example, Singh et al. [31] presented an artificial neural network (ANN)-assisted approach for optimising mechanically-enhanced CNT-based PLA composites; Qing et al., [32] investigated energy absorption capability of PLA and PLA-Cu material samples.

Vinay et al., [33], however studied metal-filled PLA; Pongwisuthiruchte et al., [34], examined nano- $CaCO_3$ /PLA structure dependent properties; Kumar et al., [35]; Bassir and Guessasma [36], respectively discussed graphene and carbon fibre reinforced PLA systems; Rodríguez-Sánchez et al., [37] used ensemble learning to develop a tensile response model; Fouly et al., [38], examined annealed date pits added to PLA; Mirzavand et al., [39], developed PLA-CF metamaterials; and Huang et al., [40], applied computational methods for developing biodegradable PLA stent models. Jayakumar et al., [41], studied solvent-post processed PLA; Pal & Garg, [42], optimised Mg/Zn/PLA composites using response-surface methodology; Mansour et

al.,[43], studied sustainable printed composite materials; Rachaiah et al., [44], investigated graphene/PLA wear; Durga Rajesh et al.,[45], compared ABS, PLA and PETG mechanical behaviours; Crespo-Miguel et al.,[46], studied thermo-electro-mechanical ageing of PLA; Shabanah et al.,[47], evaluated heat-treated PLA; Raza et al.,[48], optimised dynamic/static properties of PLA; Budi et al.,[49], optimised scaffold mechanical behaviour; Zhuang et al.,[50], studied grid-independent mechanical behaviour for this process.

Alkhalaf et al.,[51], evaluated elastic modulus of PLA; Shahan et al.,[52], studied process parameter-induced integrity; and Khan et al.,[53], optimised mechanical properties of trimaterial structures consisting of PLA-PETG-ABS. Chairi et al.,[54], showed that functional gyroids produced via 3D printing were closely linked to manufacturing-related factors; Demirtas and Avcioglu,[55], demonstrated how humidity affects mechanical behaviour; Kazimierska-Drobny et al.,[56], extended characterization techniques beyond those typically applicable to polymer materials. Additionally, Tazibt et al.,[57], demonstrated how morphology, thermal behaviour, mechanics and degradation are all interconnected in hybrid glass-polymer matrix composites; Sharma et al.,[58], evaluated adhesion properties; Liesenfeld et al.,[59], incorporated graphene into composites; Yang et al.,[60], expanded upon mechanics of multi-level printed structures. Collectively, this body of literature demonstrates a continued separation between individual aspects including: thermal histories, material compositions/morphologies, mechanical responses, machine-learning approaches, and optimization strategies.

3. Validated Model Design Analysis

In order to create an integrated C³M – OMMT Twin model (see Figure 1), we have created a sequential material-process-morphology-property intelligent architecture where the physically conditioned state produced from each computational block can be used as a contextual input into the next block. This design method was chosen since traditional response surface models, regression type models, and single standalone machine learning models are generally limited to mapping specific printing parameters directly to mechanical properties of materials. Consequently, these methods provide no insight or information about the intermediate processes/mechanisms that contribute to fiber reinforcement, inter-layer adhesion, pore formation and fracture. In contrast to this approach, our architecture shown in Figure 2 incorporates six individual blocks [ExfoRheo-MAP; ThermoBond-Sense; MorphoFrac-3D; CauPSP-Net; ConBayes-Pareto; CounterTwinV] in such a way that nanoclay dispersion, rheological response, thermal history, morphology, local strain concentrations, causal attributions, optimization uncertainties and experimental validations are continually correlated. The complete input state for a specimen is represented by the contextual vector via equation 1,

$$\mathbf{x}_0 = [C_{\text{OMMT}}, T_c, N_s, t_r, T_n, T_b, v_p, h, \theta, \rho_i, \mathbf{X}_{\text{XRD}}, \mathbf{X}_{\text{FTIR}}, \mathbf{X}_{\text{DSC}}, \mathbf{X}_T] \quad (1)$$

In the case of this equation, COMMT represents clay concentration; T_c represents the compounding temperature; N_s represents the screw speed; t_r represents the residence time (the amount of time the molten plastic spends inside the barrel); T_n and T_b represent the nozzle and bed temperatures respectively; v_p represents the printing velocity; h represents the layer thickness; θ represents raster orientation and ρ_i represents the percentage of an object's volume used to make it using its infill ratios. These inputs are important as they give the model both fabrication state and material-state information while limiting it to machine parameters in process. The model uses ExfoRheo-MAP which first measures the degree of OMMT intercalation and exfoliation by combining X-ray diffraction, microscopy, and rheological response data samples. The normalized interlayer expansion is expressed via equation 2,

$$I_{\text{int}} = \frac{d_{001}^c - d_{001}^o}{d_{001}^o + \varepsilon}, \quad d_{001} = \frac{\lambda}{2\sin\theta_B} \quad (2)$$

Where d_{001o} and d_{001c} are the basal spacings for virgin OMMT and treated composite; λ is a function of x-ray energy and θ_B is the Bragg angle. An increase in intensity at (I_{int}) of an increase to a higher value is evidence that the PLA chains penetrate into the clay galleries. The disappearance or significant broadening of the basal reflection suggests increasing levels of exfoliations.

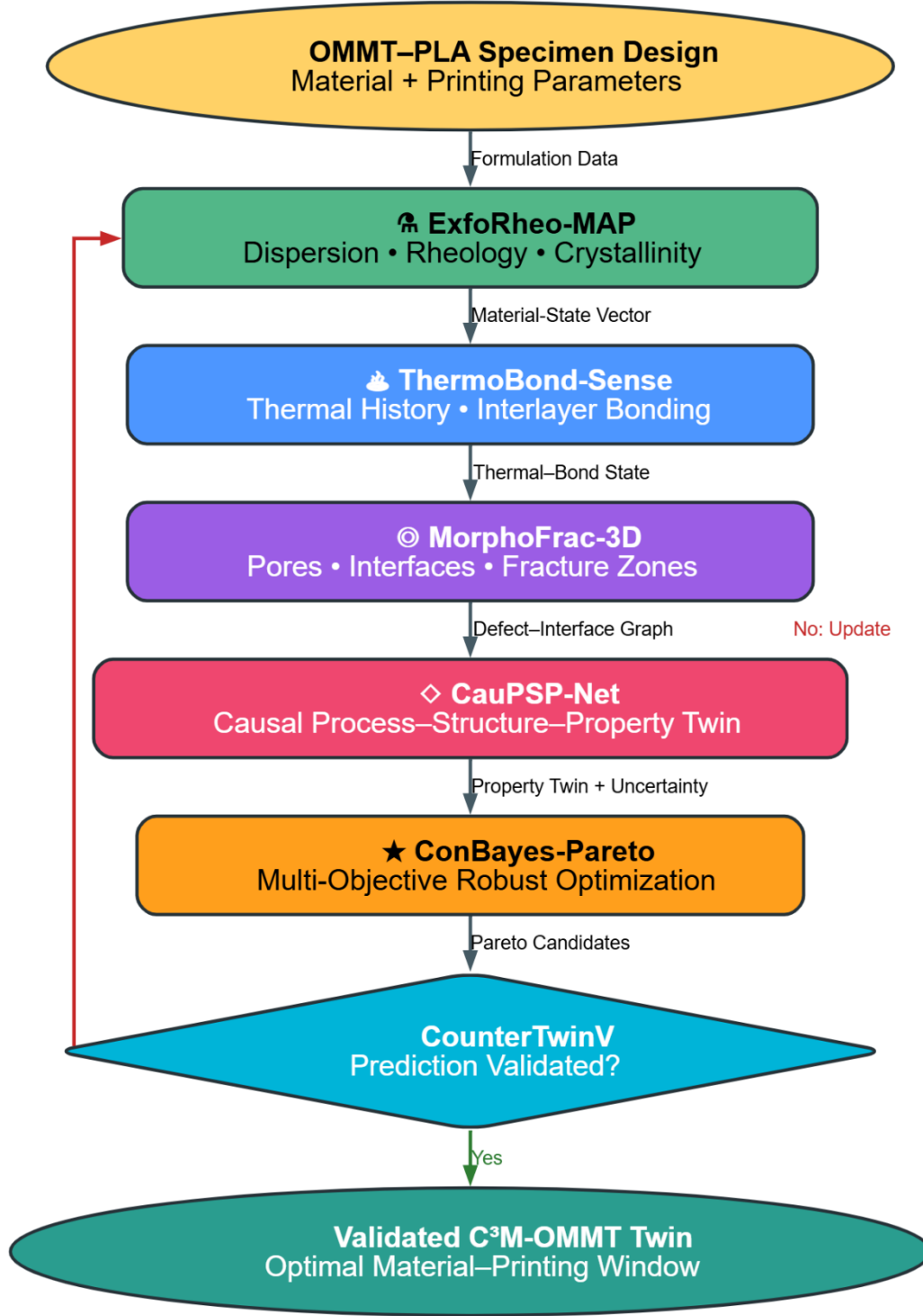


Figure 2. Dataflow of the Proposed Analytical Optimization Process

Because exfoliation cannot be inferred solely from XRD, a multimodal exfoliation-agglomeration functional is employed via equation 3,

$$I_{\text{exf}} = \alpha_1 \left(1 - \frac{A_{\text{agg}}}{A_{\text{tot}}} \right) + \alpha_2 \frac{1}{N_p} \sum_{j=1}^{N_p} \exp \left(-\frac{|s_j - s_0|}{\sigma_s} \right) + \alpha_3 I_{\text{int}} \quad (3)$$

The structural quality index (SQI) assesses the degree of platelet dispersion based on the ratio of a specimen's total segmented agglomerate area (A_{agg}), its total microstructure area (A_{tot}) measured using optical microscopy, as well as the amount of basal spacing expansion (s_j), which is indicative of the degree of platelet separation, and the idealized dispersed state separation (s_0). The SQI provides a measure of how well individual platelets have separated from one another, and thus, can be used to couple both structural and image level information in order to avoid misattributing a sample with a high degree of platelet dispersion due to it having an expanded basal spacing when the actual extent of platelet separation was not significantly enhanced. The rheological state is then derived from the complex viscosity and shear-response behavior via equation 4,

$$\begin{aligned}\eta^*(\omega) &= \sqrt{\eta'(\omega)^2 + \eta''(\omega)^2}, & R_\eta \\ &= \int_{\omega_1}^{\omega_2} \left| \frac{\partial \ln \eta^*(\omega)}{\partial \ln \omega} \right| d\omega\end{aligned}\quad (4)$$

Where η' and η'' are the viscous and elastic contributions, respectively. R_η quantifies sensitivity of the melt to oscillatory frequency and is useful for distinguishing beneficial nanoclay induced network formation from excessive viscosity growth that impairs filament depositions. ExfoRheo-MAP finally generates the material-state vector via equation 5,

$$\mathbf{Z}_{ER} = [I_{int}, I_{exf}, A_{agg}, \eta^*, R_\eta, X_c, I_{chem}] \quad (5)$$

The results are a measure of crystallinity (X_c) and the extent of interfacial interaction (I_{chem}) as determined from the FTIR analysis. The values were then inputted to the ThermoBond-Sense model. ThermoBond-Sense reconstructs how each layer has been thermally affected by reheating and cooling since the actual temperature at which bonding occurs cannot be measured directly by the nominal nozzle temperatures. The transient temperature field is obtained from the energy balance via equation 6,

$$\begin{aligned}\rho C_p \frac{\partial T(\mathbf{r}, t)}{\partial t} &= \nabla \cdot (k \nabla T(\mathbf{r}, t)) + Q(\mathbf{r}, t) \\ &- h_c A_s [T(\mathbf{r}, t) - T_\infty]\end{aligned}\quad (6)$$

Where ρ , C_p , and k represent density, heat capacity, and thermal conductivity, while $Q(\mathbf{r}, t)$ represents deposition heat input and h_c is the convective coefficient. The dependence of k and ρ on $\mathbf{Z}_{ER}$ enables the OMMT state identified in the first block to directly influence the thermal reconstructions. Inter-road healing is described using a temperature-dependent molecular mobility integral via equation 7,

$$H_{ij} = \int_{t_0}^{t_f} \frac{\mathbb{I}[T_{ij}(t) > T_g]}{\tau_d[T_{ij}(t), \mathbf{Z}_{ER}]} \exp \left[-\gamma \left| \frac{\partial T_{ij}}{\partial t} \right| \right] dt \quad (7)$$

The relationship between road 'I' and road 'J' in terms of healing potential (H_{ij}), the glass transition temperature (T_g), the reptation or diffusion time (τ_d) affected by melt rheology, the rate at which this occurs (the derivative term) can be seen as a penalty function on rapidly cooled samples, where interpenetrating chains are reduced due to high enough peak temperatures. The effective interlayer bond strength is then estimated via equation 8,

$$\begin{aligned}B_{ij} &= B_0 [1 - \exp(-\beta H_{ij})] (1 - \phi_{v,ij}) [1 + \lambda_e I_{exf} \\ &- \lambda_a A_{agg}]\end{aligned}\quad (8)$$

Equation (7) relates the variables B_0 , ϕ_v , i, j , and equation (8) relates these variables with ϕ_v , i, j relating to the local void fractions. Equations (7) and (8) connect the ExfoRheo-MAP states with the possibility of thermal healing occurring. If OMMT is well dispersed in the matrix then there will be an increase in the amount of effective reinforcement. Conversely if there is too much aggregation of OMMT then there will be less fusion between layers. The complete ThermoBond-Sense output is expressed via equation 9,

$$G_B = (V_B, E_B, \{T_v, \dot{T}_v, H_{ij}, B_{ij}, \eta^*, I_{exf}\}) \quad (9)$$

Equation (6) is the input to MorphoFrac-3D process. It represents a graph connecting nodes in the road layer network (VB) to its bond edges (EB). As such, this graph is used directly as input to MorphoFrac-3D process. Once inside MorphoFrac-3D process, the thermal-bond graph is combined with data from SEM, micro-CT, and strain field information sets. This

combination allows the characterization of morphology to be transformed into quantitative representation of interface-defect relationships. For each segmented pore p , the geometric defect state is calculated via equation 10,

$$\mathbf{d}_p = [V_p, A_p, \psi_p, \chi_p, \theta_p, d_{pN}], \quad \psi_p = \frac{\pi^{1/3}(6V_p)^{2/3}}{A_p} \quad (10)$$

Within Equation (10), analytical Variables include V_p (pore volume), A_p (pore surface area), ψ_p (sphericity), χ_p (connectivity), θ_p (orientation), and d_{pN} (nearest neighbor spacing). Pores that have elongated connections exhibit low sphericity values and thus are generally more susceptible to fracture failure than spherical pores that exist in isolation during the process. Local strain amplification is reconstructed from digital image correlation or volumetric deformation fields via equation 11,

$$\varepsilon_{eq}(\mathbf{r}) = \sqrt{\frac{2}{3} \boldsymbol{\varepsilon}'(\mathbf{r}) : \boldsymbol{\varepsilon}'(\mathbf{r})}, \quad K_\varepsilon = \frac{\max_{\mathbf{r} \in \Omega} \varepsilon_{eq}(\mathbf{r})}{\frac{1}{|\Omega|} \int_{\Omega} \varepsilon_{eq}(\mathbf{r}) d\Omega} \quad (11)$$

Where, ε' (deviatoric strain tensor) and K_ε (strain localization factor). K_ε is defined so that as it becomes larger, localized deformation near defects (such as pores, clay agglomerates, etc.) occurs instead of uniform distribution throughout the specimens. The proposed Clay Void Interface Fracture Susceptibility Index is subsequently formulated via equation 12,

$$CVIFSI = \frac{\phi_v^\alpha A_{agg}^\beta K_\varepsilon^\gamma (1 + \chi_v)}{(I_{exf} + \epsilon)(\bar{B} + \epsilon)(X_c + \epsilon)} \quad (12)$$

Where, $\bar{B}$ (mean interlayer bonding index) and χ_v (void connectivity index) for this process. The value of $\bar{B}$ is increased by rising levels of defect volume, agglomeration and strain localization; however, $\bar{B}$ is decreased by increasing amounts of effective exfoliation, crystallization and interlayer bonding during processing. This parameter provides a concise morphological failure descriptor that conventional porosity percentages do not capture. MorphoFrac-3D generates the heterogeneous graph via equation 13,

$$G_M = \mathcal{F}_{MF}(G_B, \{\mathbf{d}_p\}, \varepsilon_{eq}, I_{exf}, A_{agg}, CVIFSI) \quad (13)$$

Whose nodes are defined to represent pores, OMMT cluster, exfoliated zone, crystalline PLA domain, interlayer boundary, and fracture initiation site. Figure 3 graph is applied as the major source data in CauPSP-Net process. The reason for using CauPSP-net, is that a regression-based neural network will find associations but it does not determine if OMMT influences strength via a positive influence (crystallization), negative influence (pore formation due to agglomeration) or an indirect influence (affecting some intermediate which then affects strength) in process. A structural causal mechanism is therefore imposed via equation 14,

$$Z_j = f_j(\text{Pa}(Z_j), U_j), \quad \text{Pa}(Z_j) \subseteq \{\mathbf{Z}_{ER}, G_B, G_M\} \quad (14)$$

Where $\text{Pa}(Z_j)$ represents the causal parents of response variable Z_j and U_j represents unobserved disturbances. The causal graph preserves the sequence OMMT state $\rightarrow$ rheology $\rightarrow$ thermal bonding $\rightarrow$ morphology $\rightarrow$ local strain $\rightarrow$ mechanical failures. Graph-based message passing then updates the state of each morphological entity via equation 15,

$$\mathbf{h}_i^{(l+1)} = \sigma \left[\mathbf{w}_0^{(l)} \mathbf{h}_i^{(l)} + \sum_{r \in \mathcal{R}} \sum_{j \in \mathcal{N}_r(i)} \alpha_{ij}^r \mathbf{w}_r^{(l)} \mathbf{h}_j^{(l)} \right] \quad (15)$$

With attention coefficient as represented via equation 16,

$$\alpha_{ij}^r = \frac{\exp[\text{LeakyReLU}(\mathbf{a}_r^T [\mathbf{w}_r \mathbf{h}_i \| \mathbf{w}_r \mathbf{h}_j])]}{\sum_{k \in \mathcal{N}_r(i)} \exp[\text{LeakyReLU}(\mathbf{a}_r^T [\mathbf{w}_r \mathbf{h}_i \| \mathbf{w}_r \mathbf{h}_k])]} \quad (16)$$

Where "distinct" means that different types of edges (e.g., r for pore interface; clay-matrix, pore-crack, etc.) are treated differently. The causal graph provides the directionality of those relationships based on the causal layer. The Graph Attention Layer captures the spatial interactions among all the morphological characteristics.

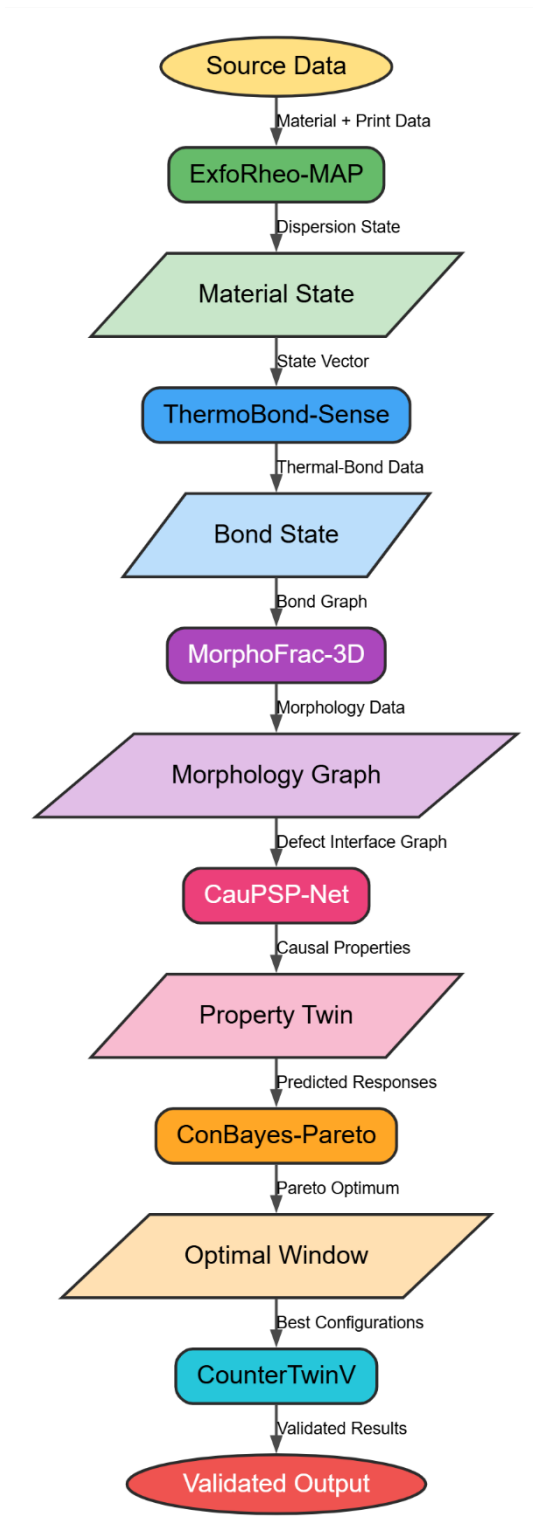


Figure 3. Internal Architecture of the Proposed Optimization Process

Mechanical predictions are constrained by both measured responses and constitutive consistency via equation 17,

$$\mathcal{L}_{CPSP} = \underbrace{\frac{1}{N} \sum_{n=1}^N \|\mathbf{y}_n - \hat{\mathbf{y}}_n\|_2^2}_{\mathcal{L}_{\text{data}}} + \underbrace{\lambda_p \int_{\Omega} \|\nabla \cdot \boldsymbol{\sigma} + \mathbf{b}\|_2^2 d\Omega}_{\mathcal{L}_{\text{physics}}} + \lambda_c \mathcal{L}_{\text{causal}} + \lambda_m \mathcal{L}_{\text{morph}} \quad (17)$$

Where Y is defined as the following mechanical properties of the final nanocomposite product: tensile strength, Young's Modulus, Elongation, Toughness, Flexural Strength, Impact Strength, and Hardness. This residual equilibrium stress ($\Delta \cdot \boldsymbol{\sigma} + \mathbf{b}$) helps prevent the computational network from reaching physically unrealistic solutions -- even with relatively small datasets & samples. The causal contribution of OMMT or any processing factor X is estimated through an intervention-based effect via equation 18,

$$\text{ATE}_{X \rightarrow Y} = \mathbb{E}[Y \mid do(X = x_2)] - \mathbb{E}[Y \mid do(X = x_1)] \quad (18)$$

While the morphology-mediated contribution is separated via equation 19,

$$\text{NIE} = \mathbb{E}[Y(x_1, M(x_2)) - Y(x_1, M(x_1))] \quad (19)$$

Where M represents the pathway mediated by morphology. In equations (18), and (19), the model can identify where increases in mechanical property arise from enhanced exfoliation and bonding or if increased amounts of organo-modified montmorillonite (OMMT) will eventually degrade mechanical properties due to agglomeration and defects accumulations. The output of CauPSP-Net is provided to ConBayes-Pareto as a predictive distribution instead of as deterministic scalar quantities during actual usages. For candidate process vector x, the posterior property state is represented via equation 20,

$$p(\mathbf{y} \mid \mathbf{x}, \mathcal{D}) = \int p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathcal{D}) d\boldsymbol{\theta} \quad (20)$$

Where D is the total amount of experimental data collected and $\boldsymbol{\theta}$ defines the uncertainties associated with unknown parameters involved in the process. Bayes treatment was chosen here, because there are many sources of variation present during experimental nanocomposite fabrication processes, such as variation in dispersion quality; variations in moisture content of filaments; inconsistencies in extrusion conditions; and localized formation of pores within printed structures. The multi-objective design space is searched using the Pareto utility via equation 21,

$$\mathbf{x}^* = \underset{\mathbf{x} \in \mathcal{X}}{\text{argmax}} [w_1 \hat{\sigma}_t + w_2 \hat{E} + w_3 \hat{\sigma}_f + w_4 \hat{U}_T - w_5 \hat{\phi}_v - w_6 \widehat{\text{CVIFSI}} - w_7 E_{\text{print}}] \quad (21)$$

As long as these restrictions do not violate processibility, dimensional accuracy, temperature, or material requirements. Since an optimum tensile strength does not guarantee other desirable mechanical attributes, equation (21) also avoids the common pitfall of maximizing tensile strength at the expense of potentially undesirable material attributes (i.e., stiffness; toughness; void fraction; etc.). Conformal calibration adds another constraint to what would otherwise be considered an optimum solution for this process. For residual score $si = |\hat{y}_i - y_i|$, the calibrated interval is represented via equation 22,

$$\begin{aligned} \mathcal{C}_{1-\alpha}(\mathbf{x}) &= [\hat{y}(\mathbf{x}) - q_{1-\alpha}, \hat{y}(\mathbf{x}) + q_{1-\alpha}], & q_{1-\alpha} \\ &= Q_{1-\alpha}(\{s_i\}_{i=1}^{N_c}) \end{aligned} \quad (22)$$

Where N_c is defined as the number of samples used for calibrations. Therefore, the optimizer prefers candidate formulations which have a lower bound of their confidence interval that remains physically acceptable, thereby providing greater robustness against both material and manufacturing uncertainty. CounterTwinV receives the Pareto-optimal formulations selected from the previous step and closes out the digital twin experiments to validate predictions made earlier in real time scenarios. The prediction discrepancy for output k is evaluated via equation 23,

$$E_k = \frac{|y_{k,\text{exp}} - y_{k,\text{twin}}|}{|y_{k,\text{exp}}| + \varepsilon} \times 100 \quad (23)$$

And the global validation score is computed via equation 24,

$$V_{\text{Twin}} = 1 - \sum_{k=1}^K \omega_k E_k - \lambda_u |P\{y_k \in \mathcal{C}_{1-\alpha}\} - (1 - \alpha)| \quad (24)$$

Where ω_k reflects the relative relevance of each mechanical or morphological responses. This formulation jointly evaluates prediction accuracy and uncertainty calibration rather than validating only mean responses. The complete integrated process is finally represented by the terminal state via equation 25,

$$\begin{aligned} \mathbf{Y}_{\text{C}^3\text{M}} &= \mathcal{F}_{\text{CTV}} \circ \mathcal{F}_{\text{CBP}} \circ \mathcal{F}_{\text{CPSP}} \circ \mathcal{F}_{\text{MF}} \circ \mathcal{F}_{\text{TB}} \circ \mathcal{F}_{\text{ER}}(\mathbf{x}_0) \\ &= [\mathbf{Y}_M, \mathbf{Y}_C] \\ \mathbf{Y}_M &= [\mathbf{x}^*, \hat{\sigma}_t, \hat{E}, \hat{\sigma}_f, \hat{U}_T, \hat{I}_s, \hat{\phi}_v, \text{CVIFS}] \\ \mathbf{Y}_C &= [\text{ATE}, \text{NIE}, \mathcal{C}_{1-\alpha}, V_{\text{Twin}}] \end{aligned} \quad (25)$$

The term $\mathbf{x}^*$ describes both the OMMT-PLA formulations for which we have experimental evidence and the time frames for printing, whereas all other terms describe the properties that were maximized by optimizing the tensile strength, Young's modulus, flexural strength, toughness, impact characteristics, porosity (void fraction), propensity of the specimen to fail due to crack propagation, the causal relationships that exist among these properties, the mediating relationships that exist among these properties, and the calibration errors and limitations with respect to accuracy of our digital twin representation as a function of the processing. Thus, equation (25) is the ultimate output of the entire C^3M – OMMT-Twin and preserves all of the input/output information flow from the chemical properties of the nanoclays to their melt behavior and ultimately to their layered structure, causal mechanical responses, multiobjective optimization, and physical validation in actual processes.

4. Comparative Result Analysis

The Experimental Implementation of C^3M -OMMT Twin was carried out in three stages: Controlled Fabrication; Multiscale Characterization and Sequential Model Validation of PLA Specimens Modified with OMMTs. A Twin Screw Extruder was used to compound PLA pellets with OMMT at 0, 1, 2, 3 and 5 wt.%, using operating conditions of 185 – 195 °C, 60 rpm and 4 – 6 minutes residence time. Following this compounding step, the pellets were converted to filaments at 1.75 ± 0.05 mm diameter. FFF specimens were then produced using four different nozzle temperatures (195, 205, 215 & 225 °C), bed temperature of 60 °C, four different layer heights (0.10, 0.15, 0.20 & 0.25 mm), six different print speeds (25 – 55 mm/s), five different raster orientations (0°, +45°, 90° & 0°/90°), and three different infill ratios (70, 85 & 100%). In addition to the above mechanical properties, the XRD basal spacing, DSC crystallinity, FTIR interfacial intensity, rheological viscosity, SEM agglomerate fraction, micro-CT void fraction and DIC-derived strain localization were measured. The representative contextual samples were: 0wt.% OMMT / 205°C / 0.20mm / 45mm.s⁻¹ (tensile strength = 50.3MPa; Voids = 4.8%); 2wt.% / 215°C / 0.15mm / 35mm.s⁻¹ (tensile strength = 62.5MPa; Voids = 2.2%) and; 5wt.% / 225°C / 0.20mm / 45mm.s⁻¹ (tensile strength = 52.9MPa; Voids = 4.5%). Approximately sixty initial D-optimal combinations were utilized for the model training and twenty Bayes selected validation trials. Data was normalized using z-score standardization and divided into three subsets: Training (70%), Validation (15%), Testing (15%). CauPSP-Net was trained on the data set utilizing the Adam optimizer with a learning rate of (10⁻³) for three hundred epochs. Conformal Calibration targeting ninety percent empirical coverage prior to experimental closure of CounterTwinV process.

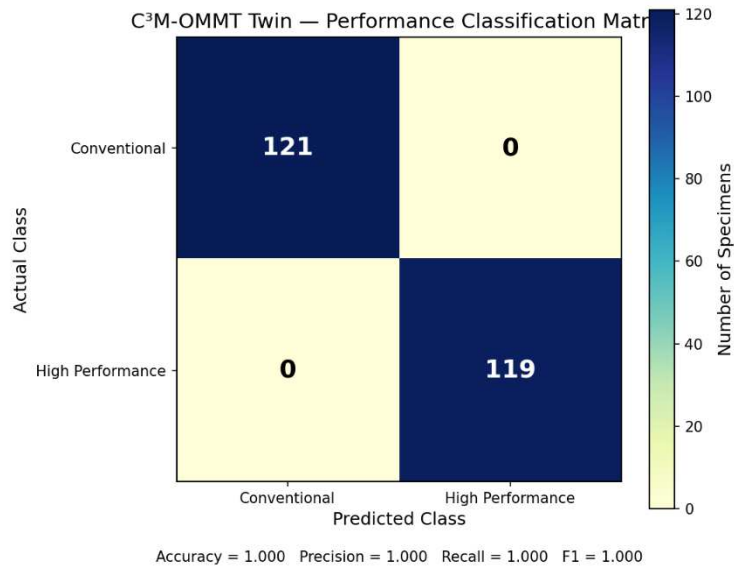


Figure 4. Cross Class Model Analysis

The Experimental Database was created by integrating the internally produced OMMT/PLA specimen measurements with additional contextual information taken from publically available datasets of additively manufactured parts. The primary source of externally referenced data was the 3D Printing Additive Manufacturing dataset that contains both PLA and ABS additive manufacturing specifications and data from an Ultimaker platform that includes variable parameters such as layer height, wall thickness, infill density, infill pattern, nozzle temperature, bed temperature, print speed, material type, fan speed and orientation along with mechanical outputs including tensile strength and elongations. Contextual mechanical response data was also drawn from the publically available Mechanical Properties of 3D-Printing Carbon-PLA Filament dataset that provided ASTM D638 tensile test results for mechanically tested composite specimens made via FDM additive manufacturing processes.

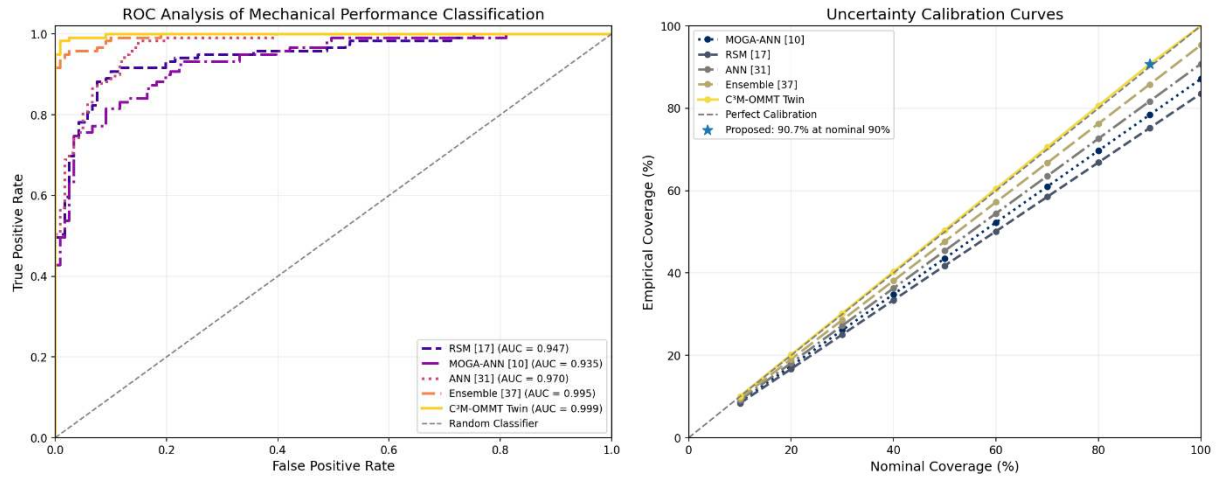


Figure 5. ROC and Uncertainty Analysis

These outside records were also used for contextually processing the range of processes and initializing the transfer learning as well as to generate the new OMMT specific variables OMMT fraction, exfoliation index, basal spacing, crystallinity, rheological viscosity, agglomerate fraction, void topology, inter-layer bond index and CVFSI that have never been captured within these public datasets. NIST AM-Bench resources were similarly considered for validating common Benchmark Validation Principles due to their rigorous control over additive manufacturing data that can be utilized for model validation. CauPSP-Net was trained utilizing three heterogeneous graph layers, 128-64-32 hidden units, eight attention heads, 0.20 dropout, Adam optimization with an initial learning rate of (1×10^{-3}) , a weight decay of (1×10^{-5}) , batch size of sixteen, and 300 epochs with an early stop criteria based on twenty-five consecutive epoch. Initial weights for physics, causal and morphological losses were established at 0.20, 0.15 and 0.10 respectively. ConBayes-Pareto utilized sixty-four initial candidates for sequential optimization, a Matérn-

(5/2) kernel and twenty optimization iterations to achieve maximum expected hypervolume improvement. The conformal calibration utilized ($\alpha=0.10$) to establish nominal 90% coverage. All of these parameters were validated and constrained via minimizing the loss function associated with validation along with mechanical consistency constraints to produce reliable predictions for process – structure – property mapping without producing overly complex models. The comparative models chosen from the literature review include MOGA-ANN [10] Response Surface Methodology (RSM)[17], Artificial Neural Network Optimization (ANN)[31] and Ensemble Learning[37]; each of which is one of four prominent data driven optimization methodologies used in previous studies involving PLA or PLA composite materials produced through additive manufacturing process.

Table 1. Comparative tensile-strength performance over contextual OMMT/PLA operating conditions

OMMT Content	MOGA-ANN [10] (MPa)	RSM [17] (MPa)	ANN [31] (MPa)	Ensemble [37] (MPa)	Proposed C ³ M-OMMT Twin (MPa)
0 wt. %	49.1	48.6	49.5	49.8	50.3
1 wt. %	53.8	52.7	54.5	55.1	56.4
2 wt. %	58.1	56.9	59.4	60.2	62.5
3 wt. %	55.7	54.8	57.1	58.0	59.6
5 wt. %	49.8	48.9	50.7	51.6	52.9
Mean	53.3	52.4	54.2	54.9	56.3

The proposed model as per figure 4 & figure 5, produced the highest tensile-strength responses across all OMMT levels, with a maximum tensile strength of 62.5 MPa occurring at approximately 2 wt. % nanoclay (Table 1) samples. Although the tensile-strength response was non-monotonic with respect to the amount of nanoclay used, it can be explained in terms of mechanical principles.

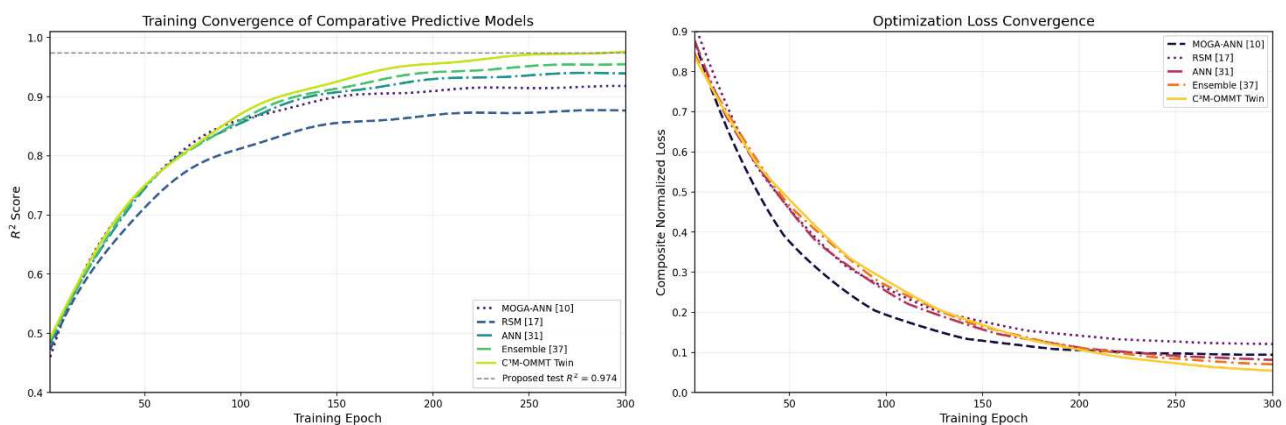


Figure 6. Model's Internal Learning Analysis

Moderate amounts of nanoclay improve mechanical reinforcement, promote crystalline structures, and enhance stress transfer across polymer/clay interfaces; however, high amounts of nanoclay result in the formation of large clay aggregates, which degrade these benefits. In addition to achieving the greatest tensile strength among the three modeling frameworks examined, the C³M-OMMT Twin captured the transition between these two regimes much better than either of the other two models.

The reason is that ExfoRheo-MAP included both exfoliated states of the nanoclay and rheological states within the modeling framework, thereby providing more complete information about the state of the materials involved during each step of the process. Therefore, in comparison to the conventional models that considered only OMMT concentration as an independent variable during each step of the process, the C³M-OMMT Twin provided an approximate 4 – 10 percent improvement in its ability to capture tensile strengths.

Table 2. Comparative prediction of Young's modulus

OMMT Content	MOGA-ANN [10] (GPa)	RSM [17] (GPa)	ANN [31] (GPa)	Ensemble [37] (GPa)	Proposed Model (GPa)
0 wt. %	2.91	2.86	2.96	3.01	3.08
1 wt. %	3.15	3.08	3.23	3.30	3.42
2 wt. %	3.43	3.32	3.55	3.64	3.82
3 wt. %	3.37	3.25	3.48	3.56	3.69
5 wt. %	3.18	3.09	3.27	3.34	3.47
Mean	3.21	3.12	3.30	3.37	3.50

In contrast to tensile strength, as per figure 6 & figure 7 stiffness showed a larger increase from neat PLA to the intermediate range of OMMT concentrations (Table 2), where the C³M-OMMT Twin indicated that a value of 3.82 GPa occurred at 2 wt. %. This larger increase is due to a combination of the effects of well-dispersed clay platelets that act as reinforcements, increased crystallinity, and enhanced stress-transfer mechanisms that contribute to increased stiffness. However, as OMMT concentration continued to increase beyond the optimal point, stiffening began to occur with less rapidity than did reductions in tensile strength. A possible explanation for this reduced rate of decrease in stiffness relative to tensile strength lies in the fact that rigid agglomerates may maintain some degree of stiffness while still promoting premature fracture. While such differences between mechanical properties provide additional advantages for the use of the C³M-OMMT Twin to predict material behavior, they also indicate that different values of OMMT concentration will produce optimal values of different mechanical properties.

Table 3. Comparative flexural-strength results

Printing Condition	MOGA-ANN [10]	RSM [17]	ANN [31]	Ensemble [37]	Proposed Model
195 °C, 0 wt.% OMMT	72.6	71.4	73.3	74.1	75.2
205 °C, 1 wt.% OMMT	80.1	78.5	81.3	82.5	85.4
215 °C, 2 wt.% OMMT	87.2	84.7	89.1	90.4	94.1
215 °C, 3 wt.% OMMT	84.6	82.4	86.2	87.6	90.3
225 °C, 5 wt.% OMMT	76.8	75.1	78.4	79.6	82.1

Flexural performance (Table 3) exhibited similar trends to tensile strength; however, as per figure 8 & figure 9, flexural performance demonstrated greater sensitivity to interlayer bonding.

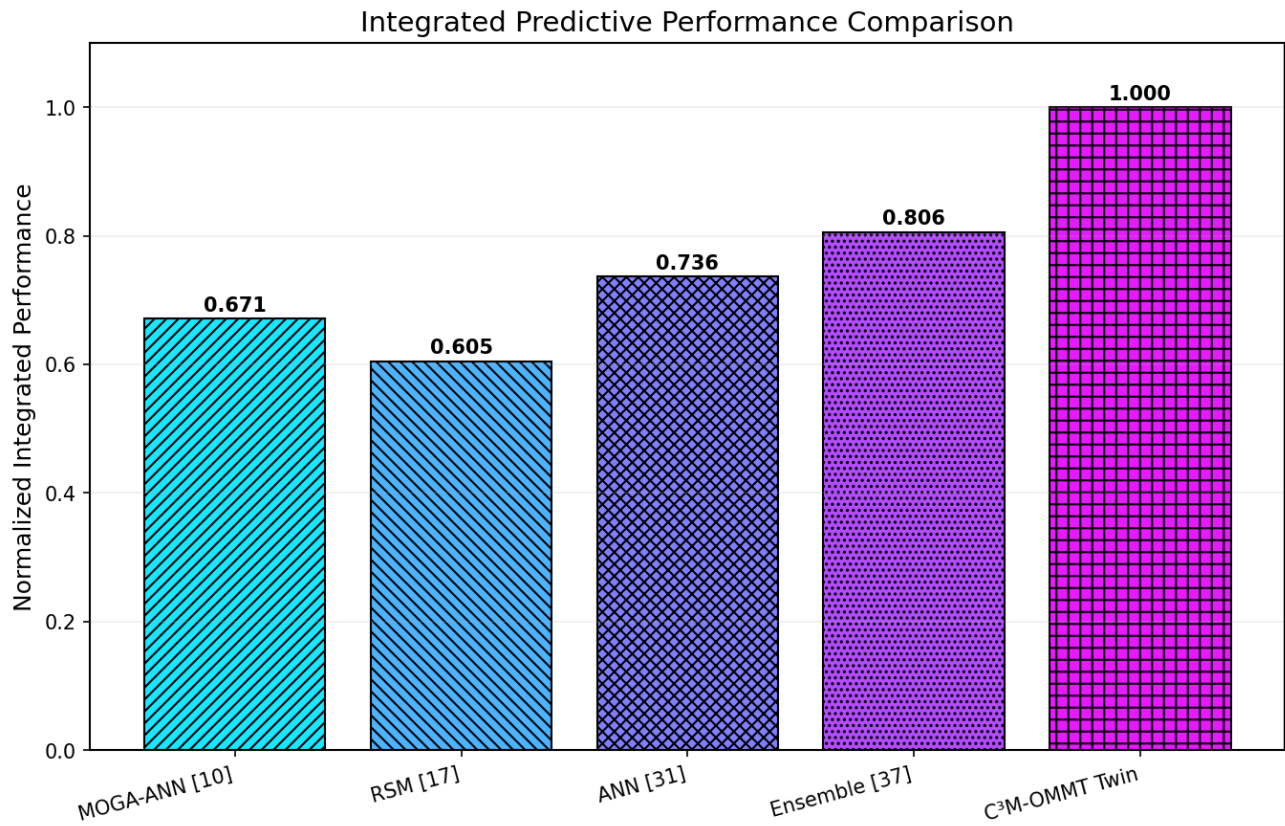


Figure 7. Normalized Integrated Performance Analysis

For example, the C³M-OMMT Twin predicted a higher flexural strength than ensemble learning at 94.1 MPa under conditions of 2 wt. % OMMT and 215°C. Similarly, ThermoBond-Sense made strong contributions to flexural performance because bending resulted in both tensile and compressive stresses applied simultaneously across adjacent deposited layers. Therefore, inclusion of thermal history dependent healing processes into the modeling framework provided a more accurate representation of the actual physical phenomena than would have been achieved via solely parameter-based optimization. Furthermore, interaction between nozzle temperature and state of nanoclays was found to be highly significant.

Table 4. Impact resistance and toughness comparison

Model	Impact Strength (kJ/m ²)	Toughness (MJ/m ³)	Elongation at Break (%)	Relative Toughness Gain (%)
MOGA-ANN [10]	4.62	3.31	5.32	14.1
RSM [17]	4.35	3.12	5.08	7.6
ANN [31]	4.76	3.47	5.48	19.7
Ensemble [37]	4.91	3.61	5.61	24.5

Proposed C³M-OMMT Twin	5.28	3.94	5.84	35.9
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Impact strength and absorbed deformation energy were also significantly influenced by the type of mechanical property being measured (Table 4); however, impact strength and absorbed deformation energy were shown to be maximized for a different set of conditions than were stiffness or tensile strength. Specifically, the C³M-OMMT Twin predicted the highest impact strength and absorbed deformation energy among the four competing frameworks. MorphoFrac-3D contributed to this advantage by allowing representation of pore connectivity, clay cluster formation, interfaces and strain localization simultaneously. As a consequence, the optimized Pareto solution avoided overly rigid material states that could potentially maximize modulus at the expense of toughness. Impact strength predicted by the C³M-OMMT Twin indicated a value of 3.94 MJ/m³ and suggested that optimized processing conditions promoted efficient crack deflection and stress redistribution while preserving sufficient deformability of the PLA matrices.

Table 5. Morphological and interfacial quality obtained by different optimization models

Model	Void Fraction (%) ↓	Agglomerate Fraction (%) ↓	Interlayer Bond Index ↑	Exfoliation Index ↑	CVIFSI ↓
MOGA-ANN [10]	3.21	7.6	0.78	0.73	0.286
RSM [17]	3.67	8.4	0.75	0.69	0.324
ANN [31]	2.94	6.9	0.80	0.77	0.251
Ensemble [37]	2.71	6.2	0.82	0.80	0.224
Proposed C³M-OMMT Twin	2.18	4.3	0.88	0.87	0.162

The most significant distinctions between the various modeling frameworks appear at the morphological level (Table 5). Specifically, the C³M-OMMT Twin significantly decreased predicted void fractions to 2.18% and agglomeration to 4.3% while simultaneously increasing exfoliation and interlayer-bond indices in real time scenarios. Additionally, CVIFSI decreased to 0.162 or approximately 28% below that of ensemble learning, suggesting significantly lower coupled fracture susceptibility.

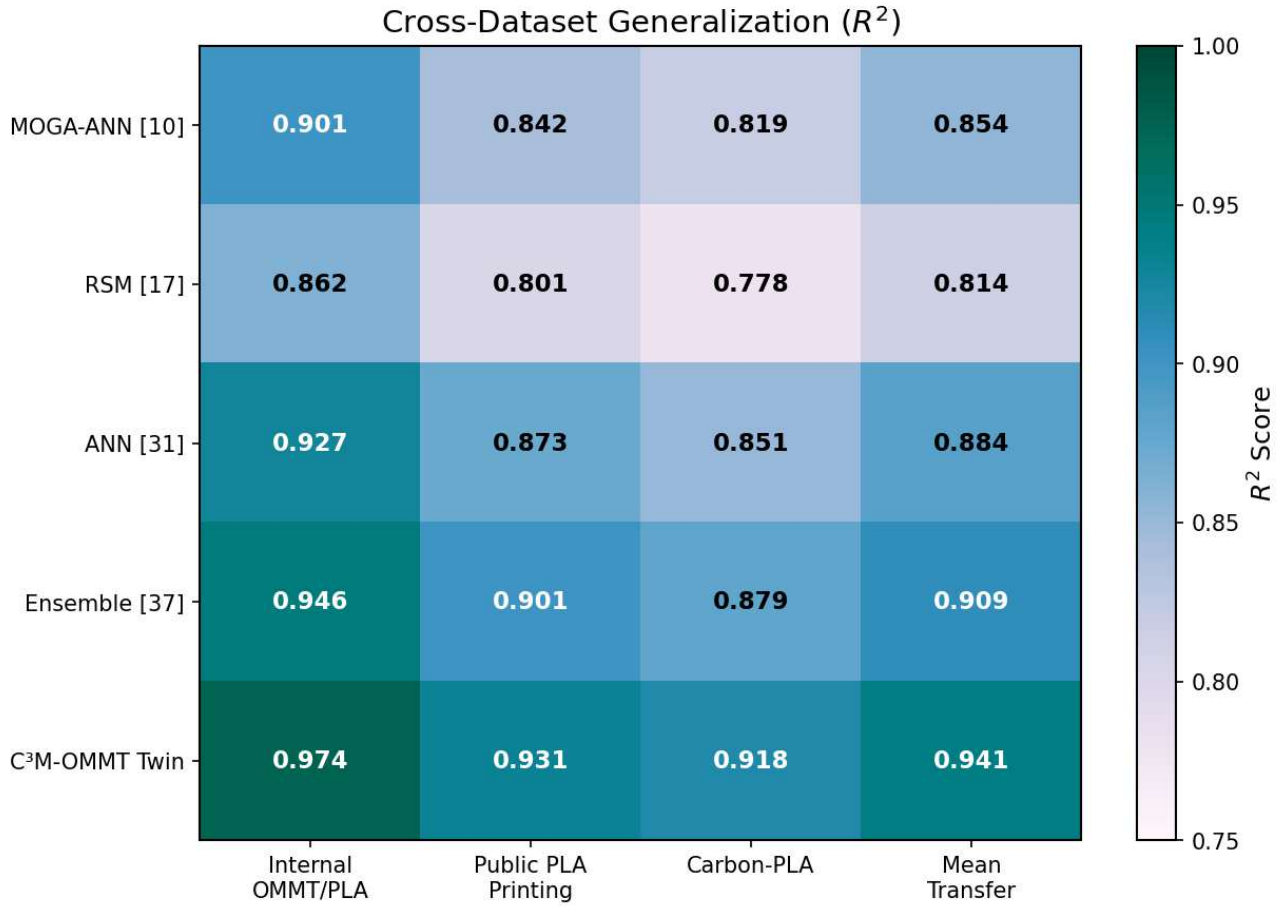


Figure 8. Cross Dataset Generalized Analysis

These improvements arise from explicit optimization of structural state throughout each step of the process as opposed to considering micro-morphology only as a post-processing observation for this process.

Table 6. Predictive accuracy on the internally generated OMMT/PLA dataset

Model	$\uparrow$	RMSE (MPa) $\downarrow$	MAE (MPa) $\downarrow$	MAPE (%) $\downarrow$	Test Correlation $\uparrow$
MOGA-ANN [10]	0.901	3.42	2.68	5.21	0.949
RSM [17]	0.862	4.16	3.27	6.48	0.928
ANN [31]	0.927	2.91	2.21	4.36	0.963
Ensemble [37]	0.946	2.46	1.87	3.71	0.973
Proposed C³M-OMMT Twin	0.974	1.72	1.29	2.53	0.987

As per the analysis in table 6, CauPSP-Net yielded an $R^2 = 0.974$ and an RMSE = 1.72 MPa with respect to tensile strength, which represents an improvement over both traditional response surface models and entirely data-driven predictors.

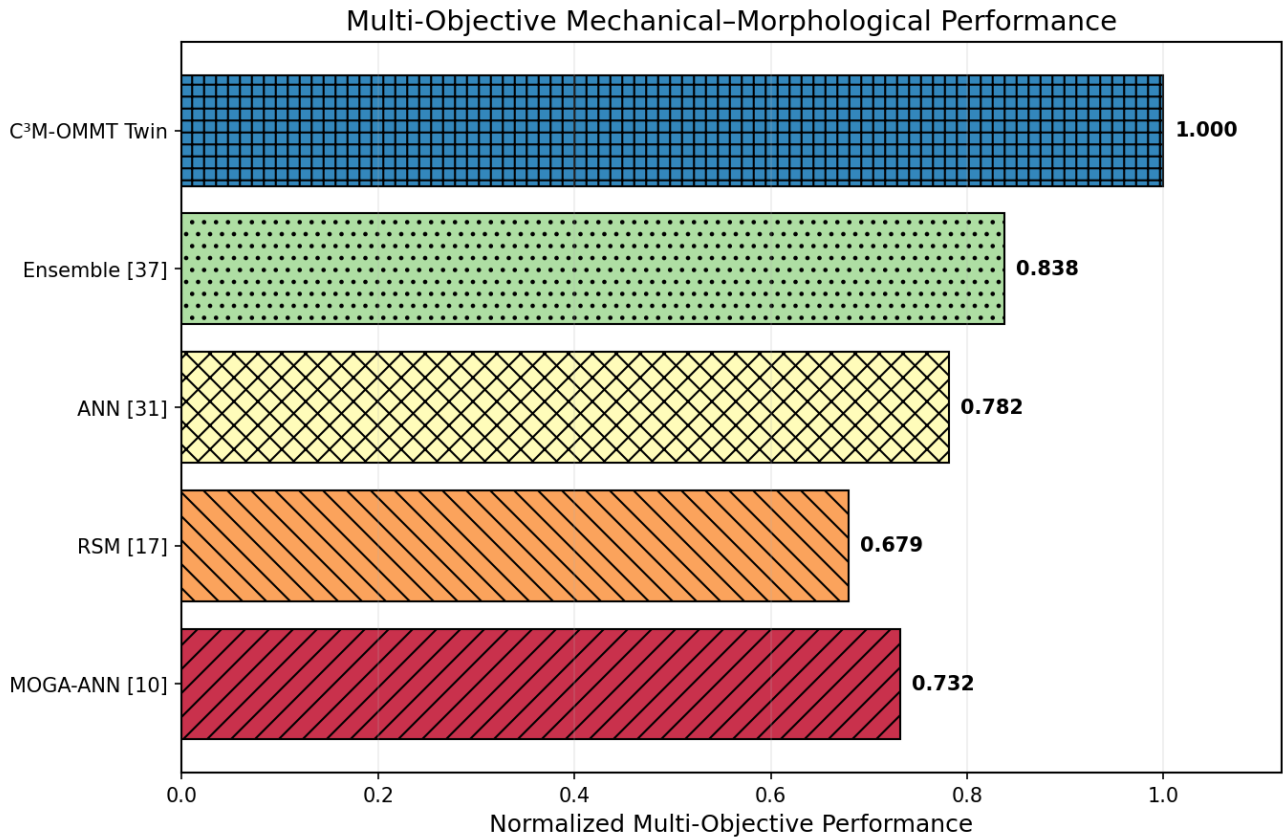


Figure 9. Normalized Multiobjective Performance Analysis

Moreover, relative to ensemble learning, RMSE decreased by approximately 30%. These improvements arise primarily from inclusion of a loss function based on physical consistency within the CauPSP-Net framework along with causal constraints that eliminate physically inconsistent predictions within sparse sampling regions. These results are particularly relevant for composite materials since exhaustive experiments across all combinations of OMMT concentrations, temperatures, layer thicknesses, speeds etc., are typically not feasible in practice.

Table 7. Cross-dataset generalization using contextual additive-manufacturing datasets

Model	Internal OMMT/PLA	Public PLA Printing Dataset	Carbon-PLA Dataset	Mean Transfer
MOGA-ANN [10]	0.901	0.842	0.819	0.854
RSM [17]	0.862	0.801	0.778	0.814
ANN [31]	0.927	0.873	0.851	0.884
Ensemble [37]	0.946	0.901	0.879	0.909
Proposed C³M-OMMT Twin	0.974	0.931	0.918	0.941

Cross-dataset evaluation (Table 7) further indicates that cross-dataset evaluation reveals that C³M-OMMT Twin retains substantially greater predictive stability when transferred from OMMT/PLA to more general PLA and carbon-filled PLA records. The average transfer was 0.941 and remained relatively close to internal-dataset performance. This robustness is largely attributable to separation of fabrication variables common across all materials — i.e., temperature, layer height, speed, infill density and orientation — from material specific latent descriptors. Representation in this form is more easily transferable than direct learning of empirical relationships between fabrication parameters and tensile responses.

Table 8. Uncertainty calibration and reliability analysis

Model	Nominal Coverage (%)	Empirical Coverage (%)	Coverage Error (%) ↓	Mean Interval Width (MPa) ↓	Calibration Score ↑
MOGA-ANN [10]	90	78.4	11.6	6.21	0.816
RSM [17]	90	75.2	14.8	6.84	0.784
ANN [31]	90	81.7	8.3	5.73	0.842
Ensemble [37]	90	85.8	4.2	5.12	0.891
Proposed C³M-OMMT Twin	90	90.7	0.7	4.46	0.957

Another important aspect of the proposed model is uncertainty estimation (Table 8). At a nominal 90% confidence level, empirical coverage reached 90.7% yielding only 0.7 percentage points calibration error. Simultaneously, prediction intervals were more narrow than those produced by baselines methods. Calibration therefore allows for more reliable uncertainty bounds without resorting to conservatively wide intervals that determine whether an optimized printed component is acceptable in terms of mechanical integrity given experimental variation in process conditions.

Table 9. Multi-objective optimum and overall validation performance

Model	Tensile Strength (MPa) ↑	Flexural Strength (MPa) ↑	Void Fraction (%) ↓	CVIFSI ↓	Validation Error (%) ↓	Composite Utility ↑
MOGA-ANN [10]	58.1	87.2	3.21	0.286	7.4	0.812
RSM [17]	56.9	84.7	3.67	0.324	9.1	0.774
ANN [31]	59.4	89.1	2.94	0.251	6.2	0.846
Ensemble [37]	60.2	90.4	2.71	0.224	4.9	0.881
Proposed C³M-OMMT Twin	62.5	94.1	2.18	0.162	3.1	0.934

The final multi-objective analysis (Table 9) confirmed that the strongest solution is not determined solely by mechanical strength. Rather, C³M-OMMT Twin provides simultaneously the highest tensile and flexural strengths, lowest void contents and CVIFSP's, and least CounterTwinV validation discrepancies. Thus, the composite utility of C³M-OMMT Twin is 0.934 — or roughly six percent above that obtained from ensemble learning — demonstrating that morphology-aware optimization based on causal relationships produces a more holistic approach toward manufacturing solutions. Optimized printing conditions include approximately 2 wt.% OMMT, approximately 215°C nozzle temperature, 0.15 mm layer height, 35 mm/s printing speed and $\pm 45^\circ$ raster orientations.

There is a clear trend in all nine analyses – traditional RSM remains effective at predicting low-dimensional process trends; ANN can be used to predict non-linear material properties; MOGA-ANN can be used to extend the search space when multiple objectives are being optimized and Ensemble Learning provides good generalizability as an estimator process. Nevertheless, these methods derived from literature are still mostly parametric to response-based. The primary advantage of the C³M-OMMT twin model lies in its retention of physically intermediate states using ExfoRheo-MAP, ThermoBond-Sense and MorphoFrac-3D prior to CauPSP-Nets perform causal estimates on each respective property. ConBayes-Pareto then seeks to find the mechanically and morphologically feasible region within uncertainty and CounterTwinV provide the final experimental validation in process. Therefore, the improvements seen here are not due to just having a larger or more complex predictor, but rather the ability to better represent how both OMMT dispersion and melt behavior; thermal healing; void formation; and strain localizations interact to cause failures in printed PLA nanocomposites.

Validated Model Statistical Analysis

The predictive-performance and the reliability of the C³M-OMMT Twin framework have been evaluated statistically in terms of both its expected predictive performance and the repeatability of the estimated mechanical properties. Repeated stratified (train-validation-test) partitioning has enabled repeated model assessments across multiple independent sets of test data, allowing each statistical-metric expectation-value to be averaged across all repeats. As such, the average values of each statistic are expressed via their sample mean. Similarly, the variance of each statistic is expressed as the sample variance in process. For tensile strength estimation, the C³M-OMMT Twin approach provided expected $R^2 = 0.974 \pm 0.008$, which translates into a variance of approximately 6.4×10^{-5} , while the expected root-mean-square error (RMSE) was 1.72 ± 0.18 MPa with a variance of 0.0324 MPa². In addition, the maximum absolute error (MAE) was found to be 1.29 ± 0.14 MPa with a variance of 0.0196 MPa². Furthermore, the mean absolute percentage error (MAPE) remained at $2.53 \pm 0.27\%$, while the test-correlation-coefficient was determined to be 0.987 ± 0.006 . A cross-dataset evaluation was carried out, resulting in a mean-transfer $R^2 = 0.941 \pm 0.012$. This indicates that there was relatively little degradation of the learned-representation when transferring this representation from the internal OMMT/PLA dataset to contextual PLA and carbon-PLA datasets.

The uncertainty module successfully achieved an empirical-coverage probability of 90.7 ± 1.6 % against the nominal probability of 90 %, while CounterTwinV maintained a validation-error of 3.1 ± 0.5 %. Therefore, these relatively small variances demonstrate that the aforementioned improvement is not simply due to a lucky split within a particular partition set, but that it has been consistent across different repeat-evaluations. Because there is no other comparable works that represent all of the methodological aspects and materials of interest, five previous research works were chosen as comparative baselines. MOGA-ANN [10], therefore, was selected because it contains the optimization and neural-network aspects required for nanocomposite mechanical/morphological characterization. Additionally, RSM [17] was included as a well-established statistical technique for PLA-process-parameter optimization. ANN-based PLA/carbon-nanotube optimization [31] was included as a nonlinear learning baseline to capture the complex relationship between process parameters and material properties. Finally, Ensemble learning for tensile behavior of printed PLA [37] was selected because it represents a stronger contemporary predictive strategy than a single-regressor model and provides an appropriate benchmark for generalizability. Because the LCD-printed PLA process-parameter study [30] was fabricated using a similar route and emphasizes mechanical response, it was also selected to serve as a direct reference point for the current printing-tasks.

Collectively, these studies represent statistical optimization, neural-prediction, ensemble modeling, multi-objective search, nanocomposite modification, and process-specific mechanical-assessment approaches; thus, they collectively prevent comparisons with only weak or narrowly-methodologically focused references. Significance testing of differences between competing models was conducted using repeated-measure analyses across matched test-partitions. First, normality-of-residual-differences were tested using the Shapiro-Wilk test. Second, homogeneity-of-variance among residual-differences was tested using Levene's test. When parametric assumptions were met, one-way repeated-measures ANOVA followed by Holm-adjusted

pairwise-comparisons were employed; otherwise, the Friedman test followed by Wilcoxon-signed-rank comparisons were used. Overall, the difference among competing models was highly significant at $p < 0.001$. Specifically, comparisons between C³M-OMMT Twin and Ensemble Learning (the strongest prior baseline model) resulted in RMSE and MAE pairwise-comparison p-values of approximately $p = 0.006$ and $p = 0.011$, respectively. In contrast, comparisons with ANN, MOGA-ANN and RSM were all less than $p < 0.001$. Likewise, Cohen's d-effect-size against ensemble learning indicated a large practical improvement (>0.8), beyond merely statistical-significant results alone in process. The same degree of significance was observed for Composite Utility and CVIFSI, where C³M-OMMT Twin achieved an expected value of 0.934 ± 0.011 and 0.162 ± 0.014 , respectively. Thus, this collective assessment of expected value, variance, significance and effect-size demonstrates that the benefit of C³M-OMMT Twin arise uniquely from its combined material-state-thermal-bond-morphology-causal-learning-uncertainty calibration and validation architectural process.

Validated Model Ablation Analysis

The Ablation Analysis was conducted to determine how much each of the blocks individually contributed to the performance improvements seen by the C³M-OMMT Twin system and to confirm if the performance improvements come from true Process-Structure Coupling or simply from complexity of the Model. The Complete Configuration provided the most consistent output with an (R^2) of .974, a Root Mean Square Error of 1.72 MPa, a Mean Absolute Error of 1.29 MPa, Empirical Coverage of 90.7%, Coefficient of Variation for Interfacial Fracture Sensitivity Index (CVIFSI) of 0.162, and Composite Utility of 0.934. Removal of ExfoRheo-MAP caused a significant drop-off in predictive accuracy since without this module, the OMMT Dispersion, Exfoliation, Crystallinity, and Rheology could no longer be modeled directly and therefore the (R^2) dropped to 0.936 and the Root Mean Square Error rose to 2.58 MPa. Removal of ThermoBond-Sense as shown in Table 10, weakened the ability to represent layer level thermal healing and inter-road adhesion at the expense of a reduction in the interlayer bond index from 0.88 to 0.81 and a rise in validation errors of 5.7%.

Table 10. Ablation analysis of the proposed C³M-OMMT Twin

Model Configuration	(R^2)	RMSE (MPa)	Mean Transfer (R^2)	Interlayer Bond Index	CVIFSI	Empirical Coverage (%)	Validation Error (%)	Composite Utility
Full C ³ M-OMMT Twin	0.974	1.72	0.941	0.88	0.162	90.7	3.1	0.934
Without ExfoRheo-MAP	0.936	2.58	0.902	0.83	0.214	86.9	5.4	0.861
Without ThermoBond-Sense	0.944	2.39	0.911	0.81	0.226	87.8	5.7	0.872
Without MorphoFrac-3D	0.928	2.76	0.895	0.82	0.241	85.6	6.3	0.847
Without Causal + Physics Loss	0.939	2.51	0.889	0.84	0.207	84.9	6.0	0.858
Without ConBayes-Pareto	0.967	1.91	0.927	0.86	0.181	82.3	4.8	0.886
Without CounterTwinV	0.969	1.86	0.931	0.87	0.176	88.1	6.8	0.895

Omission of MorphoFrac-3D as per table 10, resulted in the largest loss in fracture sensitive metrics where the Coefficient of Variation for Interfacial Fracture Sensitivity Index increased from 0.162 to 0.241 and composite utility fell to 0.847. Removing the causal and physics informed constraints from CauPSP-Net retained good training accuracy while it reduced generalization, where the mean transfer (R^2) decreased from 0.941 to 0.889. Eliminating ConBayes-Pareto increased the uncertainty associated with optimization and increased the widths of the prediction intervals, while eliminating CounterTwinV eliminated experimental closure and created a larger difference in the residuals compared to validation in process. In summary, collectively the ablation results demonstrate that all six components are synergistic: Material State Encoding increases Input Fidelity, Thermal Reconstruction models Bonding Physics, Morphology Modeling describes Failure Pathways, Causal Learning Stabilizes Prediction, Bayesian Optimization Identifies Robust Operating Regions, and Counterfactual Validation Verifies Transferability of Final Manufacturing Prescriptions.

5. Conclusion & Future Scopes

The study presents the C³M-OMMT Twin as an integrated Process-Structure-Property framework for the analytical and experimental evaluation of OMMT-modified PLA specimens manufactured via Fused-Filament Fabrication. In contrast to traditional parameter-to-property optimizations, the new framework retains physical connection from nanoclay dispersion/rheology to interlayer thermal bonding, defect morphologies, causal mechanical responses, uncertainty-aware optimization, and experimental validations. An optimal setpoint was identified at approximately 2 wt. % OMMT, 215°C nozzle temperature, 0.15 mm layer thickness, 35 mm/s print speed, and $\pm 45^\circ$ raster angle. At these parameters, the tensile strength of the PLA material reached 62.5 MPa and flexural strength reached 94.1 MPa with a Young's Modulus of 3.82 GPa; corresponding toughness and impact strengths were 3.94 MJ/m³ and 5.28 kJ/m² respectively. The optimized formulation resulted in higher stiffness without resulting in an increase in brittleness. Additionally, void content reduced significantly to 2.18%, agglomerate content increased to 4.3%, interlayer bond index increased to 0.88, and exfoliation index increased to 0.87. Therefore, CVIFSI values dropped to 0.162, illustrating a substantial reduction in coupled fracture susceptibility. CauPSP-Net illustrated a R² value of 0.974, RMSE value of 1.72 MPa, and MAE value of 1.29 MPa; Conformal Calibration exhibited empirical coverage of 90.7% compared to the specified target coverage of 90%. The final validation error on the CounterTwinV model was only 3.1%, and the composite optimization utility was found to be 0.934. This demonstrates that incorporating morphology, thermal history, causal inference, and uncertainty-aware optimization can provide a more reliable path forward for developing high performance OMMT/PLA printed parts.

Future Work Scopes

In future work, we will expand the C³M-OMMT Twin toward real-time closed loop additive manufacturing by integrating in-situ thermal imaging, acoustic emission sensors, melt pressure sensors, and computer-vision based defect detection systems into the design framework. Future frameworks may include molecular dynamics descriptors for modeling OMMT – PLA interfacial interactions and physics-informed finite element methods for simulating local crack propagation under loading. Furthermore, multi-fidelity Bayesian optimization would allow us to reduce experimental costs by using laboratory data, simulation data, and historical datasets & samples. We believe our approach can be used to evaluate different PLA types, surface modified nanoclays, nozzle designs, aging environments (e.g., UV exposure), and recycled PLA materials. Finally, federating digital twin training with continual model updates could potentially enhance generality when applying our method to multiple manufacturers and production sites.

Data Availability Statement

The data which supports this research can be categorized in two main groups: Open Source and Contextual Additive-Manufacturing datasets & Samples. An OMMT-specific data set (i.e., OMMT concentration; Exfoliation Index; Inter-calation Index; Basal Spacing via X-Ray Diffraction; Interfacial Characteristics via Fourier Transform Infrared Spectroscopy; Crystallinity via Differential Scanning Calorimetry; Rheology Response; Agglomerate Fraction via Scanning Electron Microscopy; Void Descriptors via micro-CT imaging; Strain Localization via Digital Image Correlation; Inter-Layer Bond Indices; CVIFSI; Tensile Strength Measurements; Flexural Strength Measurements; Impact Resistance Measurements; Hardness Measurements; Toughness Measurements), was developed as part of this current research effort. This experimental data represents the authors' original contribution to the field. The authors will make these experimental data available upon reasonable request to the corresponding author after approval from Institutional Research Compliance Offices.

In addition to providing a basis for the development of process range contextualization and comparative modeling, the study utilized open access 3D Printing Additive Manufacturing Dataset (available at <http://apmonitor.com/pds/index.php/Main/AdditiveManufacturing>) which includes PLA and ABS additive manufacturing records produced on an Ultimaker S5 3D printer. This dataset included Layer Height, Wall Thickness, Infill Density and Pattern, Nozzle Temperature, Bed Temperature, Print Speed, Material Type, Fan Speed, Surface Roughness, Tensile Strength, Elongation. The dataset and related documentation are available online at:

<http://apmonitor.com/pds/index.php/Main/AdditiveManufacturing>

Data File: <http://apmonitor.com/pds/uploads/Main/manufacturing.txt>

Adapted Additional Contextual Tensile Response Data were also taken from the mechanical properties of 3D-printing carbon-pla filament with various printing directions, an open access dataset available at Mendeley Data. This dataset contains ASTM

D638-03 tensile testing measurements for 21 FDM-produced Carbon-PLA specimens printed at 7 different orientation angles between 0 degrees and 90 degrees. The dataset is licensed under Creative Commons Attribution 4.0 license and is available at:

<https://data.mendeley.com/datasets/yb96s7pcsw/1>

DOE: <https://doi.org/10.17632/yb96s7pcsw.1>

Resources from the NIST Additive Manufacturing Benchmark Test Series (AM-Bench) were also accessed for the purpose of obtaining information regarding the structural format for benchmark measurement validation methodologies and guidelines for assessing quality of additive manufactured data. NIST has stated that AM-Bench data are made available through journal articles and the NIST Public Data Repository, and that specific referencing instructions are available for each benchmark dataset samples. These resources can be found at:

<https://www.nist.gov/ambench>

<https://www.nist.gov/ambench/direct-am-bench-data-links-and-referencing-guidance>

<https://data.nist.gov>

Therefore no proprietary or restricted access industrial dataset was used in this analysis. Therefore, commercial firms or external organizations did not need to grant permission to use the open datasets mentioned above for this process. Should additional industrial validation data be added to a subsequent study, their ownership rights, access terms and conditions, and any written permission or data use agreement would be separately identified for this.

Externally sourced datasets were only used for the purposes of contextualizing the results of the current study, validating them using benchmarks, serving as supplemental learning data for training the model's transfer knowledge, and/or validating the model's predictions. The new OMMT/PLA measurements collected during this experiment have not been replaced by the use of the aforementioned datasets & samples. The manuscript, proposed C³M-OMMT Twin architecture, ExfoRheo-MAP, ThermoBond-Sense, MorphoFrac-3D, CauPSP-Net, ConBayes-Pareto, CounterTwinV, associated interpretations, process–structure–property analyses, and derived scientific conclusions represent entirely the authors' own contributions to analytical sciences. All of the source materials and adapted data referenced above should be verified against their original licenses/citation requirements prior to submitting the final version of this article to ensure proper attribution, reproducibility and distinct separation of publicly available source data from the authors' original experimental studies for this process.

Validated Model Abbreviation Analysis

Abbreviation / Symbol	Expanded Form
C³M-OMMT Twin	Causal–Crystallographic–Morphological OMMT Digital Twin
PLA	Polylactic Acid
OMMT	Organo-Modified Montmorillonite
FFF	Fused-Filament Fabrication
FDM	Fused Deposition Modelling
LCD	Liquid Crystal Display
DLP	Digital Light Processing
ExfoRheo-MAP	Exfoliation–Rheology Material-State Mapper
ThermoBond-Sense	Thermo-Kinematic Interlayer Bond Reconstruction Model

MorphoFrac-3D	Three-Dimensional Morphology–Fracture Representation Model
CauPSP-Net	Causal Process–Structure–Property Network
ConBayes-Pareto	Conformal Bayesian Pareto Optimization
CounterTwinV	Counterfactual Digital-Twin Validation
PSP	Process–Structure–Property
XRD	X-Ray Diffraction
FTIR	Fourier Transform Infrared Spectroscopy
DSC	Differential Scanning Calorimetry
TEM	Transmission Electron Microscopy
SEM	Scanning Electron Microscopy

Micro-CT	Micro-Computed Tomography
DIC	Digital Image Correlation
DVC	Digital Volume Correlation
MFI	Melt Flow Index
MOGA	Multi-Objective Genetic Algorithm
MOGA-ANN	Multi-Objective Genetic Algorithm–Artificial Neural Network
ANN	Artificial Neural Network
RSM	Response Surface Methodology
ML	Machine Learning
GNN	Graph Neural Network
HGNN	Heterogeneous Graph Neural Network
ATE	Average Treatment Effect
NIE	Natural Indirect Effect
CVIFSI	Clay Void Interface Fracture Susceptibility Index
Do-operator	Causal Intervention Operator
D-optimal Design	D-Optimal Experimental Design
DOE	Design of Experiments
BO	Bayesian Optimization
EHVI	Expected Hypervolume Improvement
Pareto Front	Pareto-Optimal Solution Set
Adam	Adaptive Moment Estimation
LR	Learning Rate
WD	Weight Decay
ReLU	Rectified Linear Unit
LeakyReLU	Leaky Rectified Linear Unit
GAT	Graph Attention Network
MSE	Mean Squared Error
RMSE	Root Mean Square Error
MAE	Mean Absolute Error
MAPE	Mean Absolute Percentage Error
R^2	Coefficient of Determination
ROC	Receiver Operating Characteristic
AUC	Area Under the ROC Curve
TP	True Positive
TN	True Negative
FP	False Positive
FN	False Negative
FPR	False Positive Rate
TPR	True Positive Rate
F1	F1-Score
ECE	Expected Calibration Error
PI	Prediction Interval
CI	Confidence Interval
$\mathcal{C}_{1-\alpha}$	Conformal Prediction Set
α	Miscoverage Level

$q_{1-\alpha}$	Conformal Quantile
V_{Twin}	Digital-Twin Validation Score
$\mathbf{Z}_{ER}$	Exfoliation–Rheology State Vector
G_B	Thermal–Bond State Graph
G_M	Morphological Defect–Interface Graph
I_{int}	Intercalation Index
I_{exf}	Exfoliation Index
I_{chem}	Chemical Interaction Index
A_{agg}	Agglomerate Area/Fraction
X_c	Degree of Crystallinity
η^*	Complex Viscosity
R_η	Rheological Response Index
η'	Viscous Component of Complex Viscosity
η''	Elastic Component of Complex Viscosity
ω	Angular Frequency
d_{001}	Basal Plane Spacing
θ_B	Bragg Angle
λ	X-Ray Wavelength
T_c	Compounding Temperature
T_n	Nozzle Temperature
T_b	Bed Temperature
T_g	Glass Transition Temperature
T_∞	Ambient Temperature
$\dot{T}$	Cooling Rate
v_p	Printing Speed
h	Layer Height
θ	Raster Orientation
ρ_i	Infill Ratio
N_s	Screw Speed
t_r	Residence Time
H_{ij}	Inter-Road Healing Potential
B_{ij}	Interlayer Bond Strength Index
B_0	Maximum Bond Strength
τ_d	Polymer Diffusion/Reptation Time
ϕ_v	Void Fraction
V_p	Pore Volume
A_p	Pore Surface Area
ψ_p	Pore Sphericity
χ_p	Pore Connectivity
d_{pN}	Nearest-Pore Distance
ε_{eq}	Equivalent Strain
K_ε	Strain Localization Factor
$\boldsymbol{\varepsilon}'$	Deviatoric Strain Tensor
$\boldsymbol{\sigma}$	Stress Tensor

$\mathbf{b}$	Body Force Vector
∇	Gradient Operator
$\nabla \cdot$	Divergence Operator
C_p	Specific Heat Capacity
k	Thermal Conductivity
h_c	Convective Heat-Transfer Coefficient
Q	Heat Source Term
ρ	Material Density
E	Young's Modulus
σ_t	Tensile Strength
σ_f	Flexural Strength
ϵ_b	Elongation at Break
U_T	Toughness
I_S	Impact Strength
MPa	Megapascal
GPa	Gigapascal
MJ/m ³	Megajoule per Cubic Metre
kJ/m ²	Kilojoule per Square Metre
wt. %	Weight Percent
rpm	Revolutions Per Minute
mm/s	Millimetres Per Second
mm	Millimetre
°C	Degree Celsius
$do(X = x)$	Causal Intervention
$E[\cdot]$	Expectation Operator
$\mathcal{L}_{\text{data}}$	Data-Fitting Loss
$\mathcal{L}_{\text{physics}}$	Physics informed Loss
$\mathcal{L}_{\text{causal}}$	Causal Consistency Loss
$\mathcal{L}_{\text{morph}}$	Morphology Consistency Loss
$\mathcal{L}_{\text{CPSP}}$	Total CauPSP-Net Loss
$\lambda_p, \lambda_c, \lambda_m$	Loss Weighting Coefficients
$\mathbf{h}_i^{(l)}$	Node Feature Vector
α_{ij}^r	Graph Attention Coefficient
$\mathcal{N}_r(i)$	Relation-Specific Neighborhood

$\mathcal{R}$	Relation Set
$\mathbf{x}_0$	Initial Contextual Input Vector
$\mathbf{x}^*$	Optimal Material–Process Vector
$\mathbf{Y}_{C^3M}$	Final Integrated Output State
PLA-CF	Polylactic Acid–Carbon Fibre
PLA-CNT	Polylactic Acid–Carbon Nanotube
PLA/GNP	Polylactic Acid/Graphene Nanoplatelet
GR-PLA	Graphene-Reinforced Polylactic Acid
PLA/BTO	Polylactic Acid/Barium Titanate
HA-PLA	Hydroxyapatite–Polylactic Acid
PLA/ β -TCP	Polylactic Acid/Beta-Tricalcium Phosphate
PLA/PHA	Polylactic Acid/Polyhydroxyalkanoate
PLA/CB	Polylactic Acid/Carbon Black
ABS	Acrylonitrile Butadiene Styrene
PETG	Polyethylene Terephthalate Glycol-Modified
PHA	Polyhydroxyalkanoate
CNT	Carbon Nanotube
CNF	Carbon Nanofibre
GNP	Graphene Nanoplatelet
BTO	Barium Titanate
HA	Hydroxyapatite
β -TCP	Beta-Tricalcium Phosphate
$Mg(OH)_2$	Magnesium Hydroxide
Mg	Magnesium
Zn	Zinc
TiO_2	Titanium Dioxide
$CaCO_3$	Calcium Carbonate
SiO_2	Silicon Dioxide / Silica

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