

Physics-Informed Machine Learning for Photopolymerisation: Governing Equations, Data Assimilation and Extrapolation Limits

Embedding physical structure without freezing an incorrect model

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Abstract

Physics-informed machine learning can reduce physically implausible predictions and improve data efficiency by combining measurements with governing equations or physics-derived features. Photopolymerisation, however, couples optical attenuation, reaction kinetics, inhibition, species transport, exothermic heat generation, rheology and evolving geometry. No single simplified equation is universally valid across all resin chemistries, filler states and printing regimes. This review therefore treats physics as a set of testable constraints rather than as unquestionable truth. It defines levels of physics integration, identifies state equations that may be useful, and sets validation requirements for extrapolation beyond the calibration domain. The framework distinguishes a model that is numerically consistent with an assumed equation from one that is experimentally validated for a given photopolymer process.

Keywords: physics-informed machine learning · photopolymerisation · reaction kinetics · optical transport · heat transfer · data assimilation · extrapolation · model validation

1. Qualification problem

Physics-informed approaches are increasingly used across manufacturing because purely data-driven models can require large datasets and can generate physically implausible outputs [1]. Additive-manufacturing studies also demonstrate frameworks that fuse process-structure-property knowledge with data [2]. Photopolymerisation is a logical application, but direct validation must account for chemistry-specific reaction pathways and optical state. The central boundary is that a physics-informed model is only as correct as the physics imposed. A wrong boundary condition, omitted inhibition mechanism or invalid attenuation law can produce a model that is internally consistent and externally wrong.

2. Levels of physics integration

Physics can enter as engineered features, architectural constraints, loss-function penalties, conservation equations, boundary conditions or coupled numerical-model outputs. These levels have different interpretability and failure modes. A physics-derived feature can be audited directly, whereas a soft penalty in a neural loss may be satisfied approximately. The implementation should state which relations are enforced exactly, which are penalized and which are only used to construct inputs. This distinction matters when a model is extrapolated.

3. Optical transport and absorbed dose

Incident irradiance is not the same as local absorbed energy. Absorption, scattering, photobleaching, fillers and geometry can change the depth-dependent field (see ER-035, ER-044, ER-076 and ER-352). A simple exponential attenuation relation may be useful within a fitted regime but should not be promoted to a universal law for scattering or strongly evolving media. Physics-informed models should therefore separate measured incident conditions from inferred internal fields and retain the uncertainty of the optical model.

Table 1. Candidate physical constraints

Domain	Example relation or constraint	Qualification caution
Optics	energy attenuation / radiative transfer approximation	scattering and photobleaching can invalidate simplification
Reaction	conversion kinetics / stoichiometry	chemistry-specific mechanism
Thermal	energy balance and conduction	boundary conditions may dominate

4. Reaction kinetics and inhibition

Photopolymerisation rate depends on initiation, propagation, termination or alternative step-growth mechanisms, mobility, conversion, temperature and inhibition (see ER-030, ER-061, ER-083, ER-084 and ER-352). Radical, cationic, anionic, hybrid and click-type systems can have qualitatively different kinetic structures (see ER-064, ER-065, ER-082, ER-083 and ER-084). A common surrogate across chemistries needs either explicit regime variables or separate models. When reaction equations are simplified for computational tractability, the omitted mechanisms should be listed and the calibration domain should be defined by conversion, temperature and exposure range.

5. Heat and transport coupling

Photopolymerisation can generate heat while viscosity and reaction rate depend on temperature (see ER-351 and ER-353). Natural or forced transport, diffusion of oxygen or reactive species, and moving cure fronts can couple to the reaction. Physics-informed manufacturing reviews emphasize that thermal, chemical and fluid interactions are common sources of model complexity [1]. For thin layers under mild conditions a reduced model may be adequate; for thick sections, rapid exposure or highly exothermic systems, the same reduction may fail. Model complexity should follow a sensitivity analysis rather than a preference for maximum detail.

6. Data assimilation

Useful measurements include surface or internal temperature, spectral or Raman conversion proxies, cure depth, mass change, rheology, dimensional geometry and final properties. Data assimilation should respect where and when each measurement is taken. A surface temperature trace cannot be treated as a direct measurement of internal peak temperature without a transfer model. Multiple modalities can constrain otherwise unidentifiable parameters, but adding more data does not guarantee identifiability if parameters have compensating effects. Uncertainty-aware bridging between simulation and experiment provides a relevant adjacent example for data-assimilation design [3].

Domain	Example relation or constraint	Qualification caution
Transport	diffusion/convection	geometry and viscosity dependent
Geometry	moving cure boundary / shrinkage	threshold definitions are protocol dependent

Table 2. Model evidence ladder

Level	Evidence	Claim allowed
Fit	training data reproduced	descriptive only
Verification	implementation satisfies stated equations	numerical correctness
Independent validation	new states predicted within bounds	bounded predictive use
Boundary challenge	controlled extrapolation tested	limited transfer claim
Decision validation	performance linked to engineering acceptance	use in defined decision

7. Identifiability and parameter compensation

Kinetic constants, attenuation coefficients and heat-transfer parameters can compensate for one another when only one observable is fitted. A model may match cure depth while having the wrong internal conversion or temperature field. Parameter identifiability should therefore be assessed using multiple observables or designed perturbations. Posterior or profile uncertainty in fitted physical parameters should be retained rather than reporting a single best-fit set as intrinsic material constants.

8. Extrapolation limits

Physics-informed structure can improve extrapolation only when the enforced physics remains valid. A model trained at one wavelength cannot assume spectral invariance; a model trained on unfilled resin cannot assume the same scattering regime after adding particles; a model calibrated on thin films may fail in bulk because heat removal changes (see ER-351). Extrapolation tests should deliberately cross one boundary at a time and compare against a purely empirical baseline. Failure to improve out-of-domain behaviour is itself evidence that the imposed physics is incomplete.

9. Verification and validation

Verification asks whether the computational implementation solves the stated equations or constraints. Validation asks whether those equations represent the real process with adequate accuracy for the intended decision. Both are required. A low training loss is neither verification nor validation. Validation should use independent experimental states, uncertainty bounds and predefined acceptance metrics for the target output. If a model is used for safety or release decisions, conservative failure handling is required outside the validated domain.

10. Qualification decision boundary

Physics-informed machine learning is appropriate for photopolymerisation when it reduces data demand while keeping the governing assumptions visible and challengeable. The model should function as a structured hypothesis connecting measured states, not as a guarantee of physical truth. The strongest engineering implementation couples model-form uncertainty, parameter uncertainty and independent validation to the decision that the model is intended to support.

11. Dimensionless structure and scaling

Dimensionless groups can help identify when a physical model is likely to transfer. Ratios comparing reaction time with diffusion time, heat-generation time with thermal-relaxation time, or optical penetration depth with feature thickness can distinguish regimes even when absolute process settings differ. Such groups should be derived from the governing assumptions and validated rather than introduced merely to reduce input dimension. Scaling analysis can also show when a laboratory coupon is not representative of a printed component. A thin exposed film may be nearly isothermal while a thick enclosed volume accumulates heat; a small vat may mix differently from a production vat. Physics-informed learning should preserve these scale effects instead of absorbing them into fitted coefficients.

12. Boundary conditions as uncertain inputs

Boundary conditions are frequently the least certain part of a mechanistic model. Convective heat-transfer coefficients, oxygen concentration at a free surface, optical reflections and mechanical constraints may be poorly known. Treating them as fixed constants can make a model appear more certain than the experiment warrants. Where feasible, boundary conditions should be measured or inferred jointly with other parameters and subjected to sensitivity analysis. If the predicted decision changes across a credible boundary-condition range, additional measurement is required before using the model for qualification.

13. Failure signatures and model discrepancy

Systematic residual structure is evidence of missing physics. Residuals that change sign with depth may indicate an inadequate optical model; temperature-dependent residuals can signal omitted thermal coupling; errors concentrated near gelation can indicate a change in mobility or reaction regime (see ER-061 and ER-352). These patterns should be analysed physically rather than treated only as loss-function statistics. A model-discrepancy term can represent unresolved physics, but it must not become an unrestricted correction that

cancels conservation errors. The discrepancy model should be bounded, interpretable where possible and tested on states not used in calibration.

14. Evidence gaps and research priorities

High-value photopolymer datasets would measure internal or depth-resolved conversion and temperature together with calibrated incident optical fields, rather than relying only on final cure depth. Such data would allow competing optical-reaction-thermal models to be discriminated and parameters to be identified with less compensation. Benchmark challenges should deliberately include regime shifts: unfilled versus scattering-filled resin, thin versus bulk exposure, different wavelengths and different thermal boundary conditions. The scientific question should be whether physics-informed structure improves calibrated extrapolation, not merely in-domain fit.

References

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Competing interests

The author is Founder, CEO and CTO of 3Dresyns by Resyner Technologies S.L.; ER-405 contains no comparative recommendation between commercial products.

Data availability

ER-405 is a literature-based engineering review; no new experimental dataset was generated.