

Machine-Learning-Assisted Photopolymer Formulation: Inverse Design, Active Learning and Multi-Objective Optimisation

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Statement of Significance

Machine learning is useful in photopolymer formulation only when the optimisation problem is defined more rigorously than “predict a good resin”. Formulation variables, process parameters and measurement noise are coupled, feasible compositions occupy a constrained space, and desirable properties are usually conflicting. This review reframes ML-assisted photoresin development as a closed-loop engineering workflow linking structured experiments, uncertainty-aware surrogate models, active learning, multi-objective optimisation and printed-part validation. Proprietary 3Dresyns model architecture, training data and dosage logic are deliberately excluded.

Keywords: machine learning; photopolymer formulation; inverse design; active learning; Bayesian optimisation; multi-objective optimisation; uncertainty; vat photopolymerisation; DLP; materials informatics

Abstract

Photopolymer formulation is a constrained multi-objective problem in which liquid rheology, cure kinetics, optical attenuation, conversion, dimensional fidelity and final mechanical or functional properties interact. Machine learning can reduce experimental burden, but small datasets, correlated formulation variables, measurement noise and process-dependent labels create substantial risk of overfitting and false optimisation. Recent work has directly demonstrated ML-guided DLP-elastomer formulation and broader materials studies have established uncertainty-aware active learning and Bayesian optimisation as practical strategies for navigating expensive experimental spaces. This review defines an engineering architecture for ML-assisted photoresin development: encode chemically meaningful variables; standardise process and test metadata; use uncertainty to guide experiments; treat feasibility constraints explicitly; optimise Pareto trade-offs rather than a single score; and close the loop with printed validation. 3Dresyns customisation services are included only as implementation context, without disclosure or inference of internal algorithms.

1. Introduction

Photoresin development combines mixture design with process design. Changing a reactive diluent can alter viscosity, conversion, shrinkage and modulus simultaneously; adding a light attenuator can improve feature confinement while slowing cure; increasing functionality can raise stiffness while reducing toughness. This coupling makes the search space attractive for machine learning, but it also makes naive prediction dangerous because the measured response belongs to a formulation-process-test state rather than to composition alone [10].

The strongest current evidence moves beyond retrospective property prediction. Song and co-workers combined formulation screening, machine learning and printed validation to design DLP-printable elastomers beyond a viscosity-stretchability trade-off [1]. Okoruwa and colleagues proposed a computational-experimental photoresin design workflow for acrylates [2]. Broader materials-informatics work has established active learning, uncertainty-guided adaptive sampling and Bayesian optimisation as tools for expensive experimental spaces [3–8]. Together these studies support an iterative workflow, not an autonomous black-box formulation claim.

2. The inverse problem must be constrained

Domain	What is measured	Primary dependency	What it does not establish
Composition	Component identities and fractions.	Chemical compatibility and sum-to-one constraints.	That every numerical combination is physically mixable.
Processing	Wavelength, dose, layer, vat temperature, post-cure.	Determines conversion and printed state.	An intrinsic material property independent of printer.
Liquid state	Viscosity, stability, sedimentation, optical absorption.	Defines printable feasibility.	Final-part mechanics.
Printed state	Conversion, geometry, mechanical/thermal/functional results.	Composition plus full process history.	Causality from one ingredient alone.
Objective vector	Multiple desired properties and constraints.	Application priorities and trade-offs.	A single universally optimal resin.

Table 1. Engineering distinctions that must be preserved.

3. Data quality dominates model quality

Small formulation datasets are common because each point may require synthesis, mixing, printing, post-processing and several physical tests. Random train-test splitting can overestimate generalisation when nearby mixture compositions appear in both sets. A useful dataset should preserve replicate structure, record failed formulations, distinguish censored measurements from missing values and include process metadata. Negative results are especially important because they define the feasibility boundary.

Block	Examples	Why the model needs it	Common failure
Composition	Component identity, fraction, functionality, molecular descriptors.	Defines formulation coordinates.	Only storing product nicknames or total additive level.
Process	Printer, wavelength, dose, layer thickness, temperature, post-cure.	Separates chemistry from processing.	Mixing multiple process states under one label.

Block	Examples	Why the model needs it	Common failure
Liquid properties	Viscosity, absorbance, stability, temperature.	Defines printability constraints.	Discarding failed or sedimenting mixtures.
Printed properties	Conversion, dimensions, tensile/flexural/thermal/function.	Provides target labels.	Inconsistent specimen geometry or conditioning.
Uncertainty	Replicates, test variance, instrument limits.	Enables risk-aware acquisition.	Treating every number as exact.
Provenance	Batch, operator/date, protocol revision.	Supports drift detection.	Untraceable historical values.

Table 2. Data fields required for a defensible formulation dataset.

4. Surrogate models need uncertainty and feasibility

A surrogate model is valuable because it approximates an expensive experiment, not because it is intrinsically more accurate than physical testing. Uncertainty estimates help distinguish interpolation inside a dense region from extrapolation into poorly sampled chemistry. Lookman et al. emphasised uncertainty-aware active learning for targeted materials design [3]. In formulation work, feasibility should be modelled separately or embedded as hard constraints so that an optimiser does not repeatedly propose insoluble, unstable or unprintable mixtures.

5. Active learning and Bayesian optimisation

Active learning selects the next experiment to maximise information or progress toward a target. Bayesian optimisation adds an acquisition rule balancing exploration and exploitation [3,4]. The practical benefit is greatest when experiments are costly and the design space is structured. Polymer studies have used Bayesian and active-learning strategies for compositional search, sequence design, electrolyte formulation and plasticiser discovery [5–8]. For photoresins, the same logic should include liquid printability and printed-part validation as feasibility gates.

6. Multi-objective optimisation is the normal case

Objective A	Objective B	Why conflict arises	Appropriate output
Low viscosity	High molecular weight / network toughness.	Larger oligomers often raise viscosity.	Pareto front plus feasible processing window.
Fast cure	High optical resolution.	Greater penetration can broaden cure.	Dose-resolution trade-off map.
High modulus	High elongation/toughness.	Network density restricts mobility.	Application-weighted Pareto set.
High filler loading	Reliable light penetration.	Scattering/absorption increase with filler.	Feasible loading/process region.
Low water uptake	Hydrogel/swelling function.	Hydrophilicity drives opposite objectives.	Application-specific target rather than universal optimum.

Table 3. Typical photoresin trade-offs for multi-objective optimisation.

Collapsing multiple targets into one weighted score hides trade-offs and makes results sensitive to arbitrary weights. Pareto optimisation preserves alternatives so that the final choice can be made using application constraints [4]. This is particularly important when mechanical, thermal, optical and biological requirements are not commensurate.

7. Closed-loop validation must end on printed parts

A model recommendation is a hypothesis until the proposed formulation has been manufactured and tested using the intended process. The loop should therefore proceed from candidate generation to liquid feasibility, print calibration, specimen manufacture, post-processing, property testing and model update. The Song study is important because the loop culminated in printed elastomer validation rather than stopping at predicted composition [1]. Machine learning has also been applied to DLP pixel-intensity optimisation, showing that process variables can be learned but must remain distinct from formulation variables [9]. A similar validation standard should be used for engineering photoresins.

8. Failure modes and governance

Failure mode	Why it occurs	Detection	Control
Data leakage	Near-duplicate formulations split across train/test.	Suspiciously high validation accuracy.	Group/cluster-aware splits and external batches.
Extrapolation	Optimiser leaves sampled chemistry domain.	High uncertainty or implausible proposal.	Domain constraints and uncertainty gate.
Process confounding	Different printers/cure states mixed in labels.	Residuals correlate with process metadata.	Include process variables or stratify datasets.
Optimiser exploits artefact	Model learns measurement shortcut.	Candidate fails independent re-test.	Replicate and orthogonal validation.
Hidden feasibility failure	Composition is predicted well but cannot print.	Sedimentation, viscosity or cure failure.	Explicit feasibility classifier/gate.
Proprietary-data leakage	Publishing model details reveals recipe logic.	Reconstruction risk.	Publish framework and evidence, not internal training data or dosage rules.

Table 4. Failure modes in ML-assisted formulation programmes.

9. Minimum reporting framework

An ML photoresin paper should report dataset size and domain, composition representation, process metadata, validation split logic, uncertainty method, acquisition strategy, feasibility constraints, optimisation objectives and the number of experimentally closed-loop iterations. Final claims should be tied to independently manufactured specimens. Model architecture alone is not a sufficient indicator of scientific value.

3Dresyns implementation examples

3Dresyns offers custom material-development and selection services that illustrate where data-assisted formulation can be used operationally without disclosing proprietary algorithms.

- 3Dresyns Customization Services provides a current commercial route for requesting targeted material properties. It is implementation context for inverse material selection, not public evidence of a particular machine-learning model, training dataset or candidate-ranking algorithm [M1].
- The 3Dresyns Structured Selection Framework and structured-calibration resources illustrate the importance of coupling material selection to printer and process metadata, which is also essential for defensible machine-learning labels [M2,M3].

No internal 3Dresyns algorithm, model accuracy, formulation count, training dataset or proprietary decision logic is disclosed or inferred in this review. Product/service examples are kept outside the independent evidence chain.

10. Conclusions

- ML-assisted photoresin design should be treated as a constrained experimental optimisation problem, not an unconstrained composition generator.
- Dataset quality, failed experiments and process metadata are as important as model architecture.
- Uncertainty-aware active learning is preferable when experiments are expensive and the sampled chemistry is sparse.
- Multi-objective Pareto optimisation preserves real formulation trade-offs better than a single universal score.
- Feasibility gates for viscosity, stability, cure and printability must precede final property optimisation.
- The scientific loop closes only when model-selected formulations are printed, post-processed and independently tested.
- Commercial customisation can use these principles without requiring publication of proprietary training data or dosage logic.

Limitations

The review focuses on methodological principles and selected polymer/materials examples rather than benchmarking algorithms. Because most industrial formulation datasets are proprietary, public studies remain relatively small and domain-specific.

Author contributions

Juan Seguro: conceptualisation, literature synthesis, engineering framework, writing and critical review.

Competing interests

The author is affiliated with 3Dresyns by Resyner Technologies S.L. Commercial 3Dresyns materials are identified only as implementation examples supported by controlled product documentation. They are not treated as independent peer-reviewed evidence and no proprietary formulation composition is disclosed.

Data availability

No new experimental dataset was generated for this review. Scientific statements are attributed to the cited literature and standards; commercial examples are separated from the independent evidence base.

Company information

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