

Uncertainty Quantification for Data-Driven Photopolymer Models: Aleatoric Variation, Epistemic Gaps and Decision Calibration

From prediction intervals to engineering action thresholds

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Abstract

Data-driven photopolymer models are often reported using mean prediction error, yet engineering decisions depend on whether uncertainty is correctly calibrated at the point where an action is taken. This review separates aleatoric variation, epistemic uncertainty, measurement uncertainty and model-form uncertainty; explains why these terms are not interchangeable; and connects uncertainty estimates to accept, test-more, defer and reject decisions. Recent materials-science studies show the importance of uncertainty-aware model transfer and calibration, but photopolymer models require additional state control because formulation, cure and post-processing create strong domain shifts. The review proposes calibration tests, out-of-distribution gates and non-compensatory decision rules so that uncertainty is used to limit claims rather than decorate predictions.

Keywords: uncertainty quantification · photopolymer model · aleatoric variation · epistemic uncertainty · calibration · out-of-distribution · decision threshold

1. Why point accuracy is insufficient

A model can have a low average error while being dangerously overconfident in a narrow but important region. Engineering decisions therefore require both a prediction and an assessment of when that prediction should be trusted. Materials-characterisation work has explicitly combined prediction with uncertainty and out-of-distribution detection [1]. Photopolymer datasets make this difficult because replicate scatter, batch variation, instrument uncertainty and unobserved state changes can all contribute to error. Treating the residual variance as one undifferentiated quantity hides which part can be reduced by more data.

2. Aleatoric variation

Aleatoric variation describes irreducible or practically unresolved variation in the observations under a stated process. Examples include specimen-to-specimen variability, stochastic defect occurrence and repeatability of a measurement method. It must be estimated under controlled state conditions; otherwise drift and domain change are misclassified as random noise. Heteroscedasticity is common: variability may increase near cure threshold, phase-separation boundaries or fragile geometries (see ER-026, ER-060 and ER-075). A constant-variance model can therefore be miscalibrated exactly where decisions are difficult.

3. Epistemic uncertainty

Epistemic uncertainty reflects limited knowledge of the response function because data are sparse or absent. It should generally increase away from the training domain and can be reduced by informative experiments. Active-learning strategies use this property to select new observations [2]. In photopolymer models, distance must be defined in engineering-relevant coordinates. A candidate close in encoded composition but far in wavelength, filler state or post-cure may still be epistemically distant.

Table 1. Uncertainty classes

Class	Primary source	Can more data reduce it?
Aleatoric	repeat variation / unresolved stochasticity	not necessarily
Epistemic	sparse knowledge of response	often
Measurement	instrument/method reference	improved method can reduce
Model-form	incorrect functional structure	requires model change
Domain shift	new state distribution	requires transfer evidence

4. Measurement uncertainty

Measurement uncertainty belongs to the evidence-generating process. Irradiance calibration, balance resolution, dimensional metrology, mechanical testing and spectral processing each contribute. This uncertainty should be propagated or represented separately when training and validating the predictive model. A narrow model interval is not credible if it is smaller than the uncertainty of the reference measurement used to assess it.

5. Model-form and domain uncertainty

Model-form uncertainty arises when the chosen functional family cannot represent the process. Domain uncertainty arises when the target data distribution differs from the training distribution. Neither is guaranteed to be captured by standard predictive variance. Out-of-distribution tests should therefore accompany uncertainty calibration. If the model is not designed to recognise a domain shift, confident extrapolation can occur silently.

6. Calibration

Calibration asks whether stated probability or interval coverage matches observed frequency under the evaluation distribution. Recent work on machine-learned materials models demonstrates that uncertainty estimates can be recalibrated and that calibration quality is separable from point accuracy [3]. Calibration should be evaluated globally and by relevant subgroups: chemistry family, printer, wavelength, batch, geometry and property regime. Aggregate calibration can conceal systematic undercoverage in one subgroup.

Table 2. Decision use of uncertainty

State	Evidence pattern	Engineering action
Supported	low calibrated uncertainty; in domain	candidate may proceed
Resolvable	moderate uncertainty; informative test exists	run targeted experiment
Unsupported	OOD or uncalibrated	defer / do not claim
Failed	constraint violated	reject independent of objective

7. Decision calibration

Engineering action thresholds convert uncertainty into policy. A practical four-way rule is accept, measure again, defer for expert review, or reject. The thresholds should be set from the consequence of error and measurement capability, not from convenience. For a non-compensatory safety or qualification limit, uncertainty should widen the guard band rather than be traded against an unrelated high-performing property. Bayesian-optimisation literature provides an adjacent example of using uncertainty explicitly in materials-selection decisions [4].

8. Propagation through workflows

Photopolymer decisions often chain models: predicted cure state feeds dimensional compensation, which feeds expected property or service response. Uncertainty must propagate through the chain. Reporting only the uncertainty of the final surrogate loses the contribution from upstream state estimation. Correlated uncertainties should not be combined as if independent. Shared calibration sources, common specimens or common preprocessing can create covariance.

9. Reporting requirements

A publication should state uncertainty type, estimation method, calibration dataset, coverage metric, OOD test, subgroup analysis and how the uncertainty affects the decision. If intervals are empirical rather than probabilistic, they should not be described as confidence or credible intervals without justification. Failed predictions and high-uncertainty cases are valuable evidence and should remain in the record.

10. Qualification decision boundary

Uncertainty quantification adds value only when it changes what the engineering system is allowed to claim or do. A calibrated model should know when to request another experiment or decline a prediction. For photopolymer development, the most defensible use is a bounded decision aid whose uncertainty is calibrated against independent experiments and explicitly linked to action thresholds.

11. Coverage is not sharpness

An interval can achieve nominal coverage by being so wide that it is useless. Uncertainty evaluation should therefore report both coverage and sharpness, stratified by the engineering regime. The useful model is the one that achieves adequate coverage with intervals narrow enough to change decisions, not the one that maximizes a single uncertainty score. Sharpness should never be improved by excluding difficult OOD or failed cases from evaluation. Those cases define where the model must defer and are part of the qualification domain.

12. Calibration under distribution shift

A calibration procedure fitted on one batch, printer or chemistry family may lose coverage after a domain change. Recalibration can restore statistical coverage without proving that the underlying response model has transferred. Calibration and model validity are therefore separate questions. For a new domain, the first step is to test whether the model remains structurally adequate. Only then should calibration parameters be updated. Otherwise, recalibration may hide systematic model error by simply widening intervals.

13. Decision-theoretic guard bands

Acceptance near a specification limit should account for both measurement uncertainty and predictive uncertainty. Guard bands can reduce the probability that a nominal pass is actually outside the requirement, but their width should be connected to consequence and declared confidence rather than chosen ad hoc. When multiple properties are required simultaneously, joint uncertainty matters. Independent one-dimensional pass probabilities cannot be multiplied blindly when endpoints share specimens, calibration sources or latent cure state.

14. Evidence gaps and research priorities

Photopolymer publications rarely provide enough raw replicate and cross-domain data to distinguish aleatoric variation from epistemic uncertainty. Future datasets should include repeated preparations, repeated measurements, multiple batches and deliberate domain shifts with stable identifiers. Prospective calibration is especially important. A model should state its interval or deferral decision before the new experiment is revealed, then accumulate coverage statistics over time. Retrospective intervals tuned after seeing errors provide weaker evidence of decision reliability.

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Competing interests

The author is Founder, CEO and CTO of 3Dresyns by Resyner Technologies S.L.; ER-406 contains no comparative recommendation between commercial products.

Data availability

ER-406 is a literature-based engineering review; no new experimental dataset was generated.