

Active Learning Under Safety and Manufacturability Constraints: Candidate Selection, Feasible Regions and Stopping Rules

Adaptive experimentation that treats infeasibility as evidence rather than noise

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ER-407 · Engineering Review · Version 0.1 · 7 October 2026

Abstract

Active learning can concentrate experiments where new data are most informative, but unconstrained selection is inappropriate for photopolymer development because candidate formulations can be unstable, unmixable, incurable, unsafe or incompatible with equipment. This review defines a constrained active-learning architecture with separate models for scientific response, feasibility and operational risk. It distinguishes uncertainty sampling from objective optimisation, retains failed experiments as boundary information, and introduces stopping rules based on decision resolution and value of information. Published materials-discovery and adaptive-manufacturing studies demonstrate the power of uncertainty-guided experimentation, while safety-focused SDL literature emphasises the need for bounded autonomy. The photopolymer implementation proposed here requires pre-authorised search domains, hard interlocks and independent confirmation.

Keywords: active learning · constrained experimentation · photopolymer formulation · feasibility · safety · manufacturability · stopping rule · value of information

1. Active learning is not unrestricted exploration

Active learning chooses measurements that are expected to improve a model or decision [1,2]. In a laboratory, however, not every mathematically interesting point is physically or operationally admissible. Photopolymer formulation has hard limits associated with handling, reactivity, optical exposure, temperature, viscosity and chemical compatibility. The selection algorithm therefore operates inside an authorised experimental envelope. Outside that envelope, the correct response is not a lower acquisition score but an explicit prohibition or human-review gate.

2. Separate response and feasibility models

A response model estimates the property of interest; a feasibility model estimates whether the experiment can be prepared, processed and measured. Treating failed experiments as missing data removes exactly the observations that locate the feasible boundary. Feasibility may itself have levels: physically mixable, dispensable, printable, measurable, and application-feasible. A candidate can pass early levels and fail later ones.

3. Safety constraints

Safety-focused SDL literature argues that autonomy requires engineered safeguards, risk assessment and defined authority [3]. For photopolymer work, relevant constraints include hazardous component classes, maximum temperature, exotherm, permitted irradiation hardware, ventilation and waste handling. Safety variables should be enforced independently of predicted performance. A candidate with exceptional predicted properties does not earn permission to violate a safety boundary.

Table 1. Candidate-status logic

Status	Meaning	Controller action
Admissible	inside hard safety/equipment limits	score by acquisition rule
Uncertain feasibility	inside safety limits but manufacturability unknown	boundary/diagnostic test
Infeasible	known process/manufacturing failure	record and exclude
Prohibited	outside safety/authority envelope	do not execute

4. Manufacturability constraints

Viscosity, sedimentation, phase stability, recoating, cure window, adhesion and washability can determine whether a formulation can be processed (see ER-033, ER-034, ER-036 and ER-075). These constraints may be state-dependent: a formulation printable at one temperature or layer thickness may be infeasible at another. The active learner should therefore define feasibility jointly with process state rather than label a formulation globally printable or nonprintable.

5. Acquisition strategies

Uncertainty sampling is appropriate when the goal is model learning; expected improvement or related criteria are appropriate when the goal is optimisation; value-of-information criteria can focus experiments on a decision boundary. The acquisition function should match the stated question. Published adaptive manufacturing work demonstrates batch selection of feasible process configurations [4]. The lesson for photopolymers is methodological, not a direct performance transfer: feasibility and domain knowledge can be built into adaptive selection. Bayesian optimisation provides an adjacent framework for balancing information gain and candidate selection [5].

6. Boundary-focused experimentation

Near a feasibility boundary, replicate experiments are especially important because classification can be sensitive to small state variations. A single failure should be investigated for whether it reflects the candidate, the executor or the measurement system. Boundary experiments should use conservative stepping and pre-defined abort criteria. The objective is to map the transition, not to force execution of increasingly risky candidates.

Table 2. Stopping criteria

Criterion	Evidence required	Risk if used alone
Target reached	independent confirmation	local optimum
Low value of information	calibrated uncertainty and decision model	misspecified utility
Stable boundary	replicated boundary points	unseen disconnected feasible region
Experiment budget	none	arbitrary scientific endpoint

7. Drift and nonstationarity

Active learning assumes that new observations are comparable with prior ones. Resin ageing, environmental drift, hardware maintenance or raw-material changes can violate this. Reference controls and time covariates should be used to detect nonstationarity. If drift is detected, the learner should pause and decide whether to recalibrate, segment the campaign or restart under a new state version.

8. Stopping rules

Stopping should be defined before the campaign. Possible criteria include target attainment with confirmation, low expected decision value from another experiment, stable feasible-region boundary, or no material change in the Pareto set after replicated updates. A purely numerical criterion such as small surrogate variance can be misleading if the model is confidently wrong or if the measurement system has drifted.

9. Confirmation and auditability

Final candidates should be prepared independently from the adaptive sequence and tested under locked methods. The publication should retain all executed points, failed points, rejected proposals, human interventions and constraint changes. This record allows readers to distinguish genuine experimental efficiency from hidden curation or manual rescue.

10. Qualification decision boundary

Constrained active learning is a disciplined way to spend experiments where they change a decision. Its engineering advantage depends on treating infeasibility, uncertainty and safety as first-class information. For photopolymer development, a valid autonomous campaign is therefore defined as much by what it refuses to run as by what it selects.

11. Cost-aware and multi-fidelity selection

Not all experiments have equal cost. A viscosity measurement can be fast while ageing, fatigue or chemical-resistance tests can require days or weeks. Active learning can use multi-fidelity strategies in which inexpensive screens narrow the domain before costly confirmation, but the correlation between fidelities must be demonstrated. A low-cost proxy should not be promoted to a qualification endpoint merely because it correlates with one dataset. The selection policy must retain which fidelity produced each observation and should reserve high-fidelity tests for decisions where their expected value justifies the cost.

12. Constraint uncertainty

Feasibility boundaries are themselves uncertain. Viscosity may be measured with error, printability can depend on machine state, and chemical stability may evolve with time. A candidate close to a constraint should therefore be treated as a probability distribution or guarded decision rather than a deterministic pass/fail label. Conservative acquisition can penalize candidates whose feasibility uncertainty is high, while targeted boundary experiments can reduce that uncertainty. The appropriate balance depends on the consequence of executing an infeasible experiment.

13. False efficiency and search bias

An active learner can appear efficient if the initial design already contains a near-optimal region or if experts silently restrict the search using knowledge not reported in the formal problem. Such expert knowledge is legitimate, but it should be represented as an explicit prior, constraint or pre-screen rather than hidden from the efficiency comparison. Efficiency should be reported against multiple baselines where possible and should include wall-clock time, material use and failed executions as well as the count of successful measurements.

14. Evidence gaps and research priorities

Photopolymer active-learning benchmarks should include time-dependent stability, mixed categorical-continuous variables and disconnected feasible regions. A useful challenge would require the learner to discover both a high-performing formulation and the conditions under which it remains printable after storage or temperature variation. Safety research should also test graceful failure: deliberately corrupted sensor inputs, executor faults and out-of-domain candidate proposals should cause containment and deferral rather than continued autonomous experimentation.

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Competing interests

The author is Founder, CEO and CTO of 3Dresyns by Resyner Technologies S.L.; ER-407 contains no comparative recommendation between commercial products.

Data availability

ER-407 is a literature-based engineering review; no new experimental dataset was generated.