Data-Efficient Bayesian Optimization for Improving the Functional Properties of Cellulosic Foams

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The increasing demand for sustainable materials has positioned bio-based foams as promising alternatives to petroleum-derived counterparts [1]. Nevertheless, their comparatively limited functional performance remains a key barrier to widespread replacement of conventional plastic foams [2].

Enhancing the functional properties of bio-based foams typically requires extensive experimental trials, making the identification of optimal formulations time-consuming and resource-intensive. Industrial applications often demand application-specific properties, such as mechanical stability and hydrophobicity for general packaging, or thermal stability and chemical resistance for food-related packaging. Consequently, a single universal formulation is impractical, and determining tailored compositions for each use case becomes experimentally burdensome. This challenge is further amplified by rapidly evolving material regulations in the EU and other regions, which increase the need for adaptable and efficient optimization tools.

Machine learning–driven optimization frameworks, particularly Bayesian optimization, offer a data-efficient strategy by serving as surrogate models for complex formulation problems [3]. Such approaches significantly reduce the number of required experiments while guiding the search toward compositions that meet predefined performance targets.

In this study, a Bayesian multi-objective optimization framework was developed to optimize the composition of cellulosic-based foams for targeted functional properties. The workflow begins with an initial sparse experimental dataset generated from a diverse set of formulations and corresponding material characterizations. This dataset is used to train a Gaussian processes, which then proposes new candidate compositions using Expected Hypervolume Improvement (EHVI) based on specified property objectives. The framework operates under an active learning scheme, where characterization results from newly tested samples are iteratively incorporated to continuously improve model accuracy and decision-making.

Using this framework, an optimized formulation for the cellulosic foam was identified, consisting of a specific combination of three additives: lignin, graphite, and precipitated calcium carbonate, which are individually used in industry to enhance particular properties of bio-based foams. The initial training dataset comprised only 17 samples, in which each additive was evaluated separately across different concentration levels. Despite this limited dataset, the Bayesian optimization approach proposed a formulation that demonstrated substantial performance gains. The optimized composition exhibited an approximately 90–157% increase in Young's modulus, meeting the requirements of the packaging industry depending on the measurement direction, and indicating significant mechanical reinforcement. It also showed markedly improved surface hydrophobicity, with the foam maintaining hydrophobic behavior for over 20 minutes, which is crucial for stability in packaging applications. The obtained results are iteratively incorporated into the model within the active learning loop, enabling continuous refinement of predictions and progressive improvement of subsequent formulations in line with evolving targets.

Our approach demonstrated not only a systematic framework for the optimization of material properties, but also an intelligent experimental planning strategy that enables more efficient exploration of the formulation space and progressive improvement of material performance across iterations. Importantly, the dataset employed in this study was obtained through experimental measurements, highlighting the practical relevance of the methodology and its strong potential for application in industrial R&D settings.

References

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