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Sustainable specialty chemical design through multi-objective latent-variable model inversion

Product formulation in the specialty chemicals industry requires balancing product quality, cost, and environmental impact. This work proposes a data-driven framework for sustainable formulation design based on latent-variable model inversion combined with multi-objective optimization. Partial Least Squares (PLS) models are built to relate raw-material properties and compositions to product quality within a reduced latent space. The inversion of the PLS model is then formulated as a multi-objective mixed-integer nonlinear optimization problem. The approach simultaneously optimizes three competing objectives: (i) achieving a desired product quality target; (ii) minimizing formulation cost; and (iii) maximizing environmental sustainability. The economic objective minimizes formulations unit cost combining polymer and component costs weighted by mass fractions, using proxy costs for confidentiality reasons. Sustainability is quantified through an index derived from hazard classifications using a decision-tree methodology based on the Globally Harmonised System classification and labelling of chemicals.

The methodology is applied to the formulation of unsaturated polyester resins, where multiple raw materials (polymers, reactants, and additives) must be selected and blended under compositional and statistical feasibility constraints.

The optimization generates a set of feasible non-dominated solutions, enabling the exploration of trade-offs among objectives. Results highlight that: higher mechanical performance is associated with increased cost and reduced sustainability, while more sustainable formulations tend to be more expensive and may slightly reduce product quality. Furthermore, the proposed methodology supports informed decision-making by quantifying these trade-offs and identifying alternative formulations that maintain good product performance while improving cost and environmental impact.

Special/ Invited session

Classification

Both methodology and application

Keywords

AI, product formulation, PLS model inversion, resins

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Track Classification: AI: Machine Learning and Predictive Analytics