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A Streamlit-Based Platform for Ternary Solvent Solubility Modeling and Crystallization Process Design

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ABSTRACT

Crystallization design in pharmaceutical development is commonly supported by modeling approaches for single-solvent and binary solvent systems. In some cases, ternary solvent mixtures are desirable due to better impurity purge. However, this benefit can be offset by increased operational and analytical complexity arising from the multicomponent solvent composition, which can limit systematic exploration and broader adoption of ternary crystallization strategies during process development. To address this challenge, a user-accessible analytics platform has been developed using Streamlit to enable ternary solvent solubility modeling and crystallization process design within an integrated workflow. The application allows users to upload experimentally measured solubility data for ternary solvent systems via a web-based interface. Upon data import, the software automatically fits the data to five semi-empirical ternary solubility models using nonlinear regression. Model performance is evaluated using statistical goodness-of-fit metrics. The app outputs parity plots and fitted parameter values for all five candidate models, and an interactive ternary solubility for the best model. This approach enables transparent model comparison and supports informed selection of solubility correlations best suited for a given system, rather than reliance on a single prescribed model. The selected solubility model parameters are subsequently fed into a crystallization design module tailored to process-relevant decision making. The experimental data and fitted solubility surfaces are visualized on ternary solubility diagrams, facilitating assessment of solvent composition effects that may occur due to process variability. Building on these correlations, a downstream crystallization mapping tool enables users to explore solvent composition trajectories representative of realistic process operations, such as incremental antisolvent addition. By targeting user-specified final solubilities, the platform supports estimation of key performance indicators in pharmaceutical process development such as crystallization yield and mother liquor losses. In summary, this work demonstrates how streamlined process analytics and model selection tools can reduce the practical complexity associated with ternary solvent crystallization, enabling data-driven design decisions that leverage the impurity-purging advantages of multicomponent solvent systems in pharmaceutical manufacturing.