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From Mechanistic Model to Digital Twin: A Framework for Real-Time Optimization of Ethanol Production In S.Cerevisiae

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ABSTRACT

The transition to smart bioprocessing requires control strategies capable of managing the nonlinear dynamics and limited observability in industrial fermentation. In this work, we developed a fed-batch digital twin process for ethanol production by Saccharomyces cerevisiae via combining a mechanistic model with advanced data assimilation to achieve robust Nonlinear Model Predictive Control (NMPC). Recursive Bayesian state estimators have been developed to overcome nonlinearities of the biological models both anaerobic and aerobic, complex metabolic shifts, batch-to-batch parameters variability, and lack of biomass online measurements. Observers (soft sensors) were constructed and benchmarked for computational tractability and statistical accuracy, including Extended (EKF), Ensemble (EnKF), and Particle Filters (PF), They achieved best overall MSE improvements over the mechanistic model; The closed-loop framework showed a robust performance tested by parametric model-plant mismatches, and heteroscedastic measurement noise.