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A "real-time" sequential hybrid modeling approach to monitor and forecast key process variables in ethanol fermentation using lignocellulosic feedstocks.

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The operation of fermentation-based fuel and chemical production processes that utilize lignocellulosic substrate can be challenging due to the inherent variation in the feedstock. The failure to account for these variations in feedstock not only results in poor fermentation performance but also gives rise to scheduling challenges in both up-stream and down-stream of the fermentation, resulting in overall loss of production efficiency and equipment utilization.

This study addresses this practical need by developing a cost-efficient process monitoring solution based on on-line spectral data collected with an ATR-MIR spectrophotometer which is used in a novel sequential linear data-driven and a mechanistic model to monitor and predict the consumption of substrates and the production of ethanol in real time. Specifically, this approach consists of an iterative calculation of the probability distribution of the concentration of glucose, xylose and ethanol. At each time step, the concentration of glucose is calculated based on a partial least squares regression model that correlates spectral measurements and glucose concentration. This information is then used to make prediction of xylose and ethanol concentrations based on a mechanistic model describing the kinetics of the fermentation at each time step. The uncertainty associated with both experimental data and parameter estimation is then propagated through the model using 100 Monte Carlo simulations, which calculates the probability distribution for the predictions of glucose, xylose, and ethanol. This approach was

successfully validated at lab-scale in three cellulose-to-ethanol fermentations with different initial conditions. The sequential model was updated every 15 minutes allowing to re-estimate the state variables and to predict the course of the fermentation in real-time. Glucose and ethanol were successfully predicted with a 95% CI of 1 g/L, and xylose was predicted with a 95% CI of 5 g/L. In addition to monitoring the progress of the fermentation, it was possible to define end-point criteria for the fermentation based on the predictions made by the mechanistic model. This method allows to operate the fermentations accounting for substrate variations and opens up the opportunity for the implementation of model-based control schemes.