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Implementation of in-line PLS model and sensor fusion for real-time reaction monitoring

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Real-time monitoring of chemical processes is key for optimizing yield, preventing out of specification product, and improving overall process efficiency. Process analytical technology (PAT) tools, such as near-infrared and infrared (IR) spectroscopies, provide a real-time window into chemical processes, enabling non-destructive monitoring of analyte concentrations, and reducing dependance on labor-intensive off-line analytical methods (e.g., gas chromatography). Nevertheless, there are cases where the application of spectroscopy alone can be challenging, e.g., when analyte concentrations reach the method limit of quantification (LOQ). Moreover, PAT alone cannot predict future time steps of the process.

The present work showcases the application of in-line monitoring coupled with a hybrid modeling approach for chemical reaction. An IR probe is submerged in solution within the reactor and a Partial Least Squares (PLS) model developed to predict in real time the concentration of the limiting reagent directly from IR spectra. The PAT is then combined with the process mechanistic knowledge in a Kalman filter, which has previously proven to reduce predictions uncertainty [1]. Here, a second-order reaction kinetic model with two reagents forming one insoluble product was assumed. No additional calibration effort is necessary in this case because the reaction kinetic model is continuously reparametrized during the reaction, based on the PAT predictions. The predictions of these two models were combined with the application of the Kalman filter to optimize estimates.

The application was successfully implemented at the laboratory scale where the hybrid model was able to capture the physics of the reaction, providing end-point determination with higher degrees of accuracy. This strategy not only reduced the PAT LOQ and improved production scheduling but also reduced turnaround time and analytical costs. Additionally, it eliminated the need for manual sampling, mitigating the risks of operator exposure to the material.

References
[1] D. Krämer and R. King, “spectroscopy and a sigma-point Kalman filter,”J. Process Control, 2017.

Type of presentation

Contributed Talk

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