

# “Looking Deeply into Catalytic Systems: Mechanism and Optimization using Laboratory Automation”

## Abstract

Discovery and optimization of new reaction methodologies requires a detailed analysis, beyond simple end-point metrics, such as yield at a fixed time point. The most complete analysis involves acquiring reaction progress data, which allows multiple components to be visualized from a single experiment. This would include the transient concentrations of starting materials, intermediates, catalyst complexes, byproducts and products. These measurements provide crucial data related to catalyst robustness, reaction chemoselectivity and reaction stability.

While full reaction progress analysis represents the best case, building and validating robust analytic methods requires significant effort. Recently, we have developed a set of tools, which leverage laboratory automation to facilitate acquiring reaction progress data. In addition, our approach employs multiple orthogonal techniques that serve to cross-validate and reinforce each other.

This presentation will outline how our approach allows detailed kinetic analysis to become a routine objective for any reaction system. This includes being able to acquire accurate reaction progress data from chemical systems involving heterogeneous components, high pressure, air/water sensitive species or extreme temperatures. Current progress on model systems will be discussed.