

Mechanistic Understanding of Complex Catalytic Reactions Through In-situ Monitoring

Donna G. Blackmond PhD NAE NAS FEng FRS
Professor and John C. Martin Endowed Chair in Chemistry
Scripps Research, La Jolla CA

Reaction progress kinetic analysis streamlines mechanistic understanding and pharmaceutical process development by exploiting the extensive data sets available from accurate in-situ monitoring of global reaction progress under practical operating conditions. Temporal concentrations replace discrete initial rate measurements, permitting rapid extraction of key information about the reaction's driving forces and its robustness. The TSR protocol extends this concept by making temperature a continuous variable along with concentrations, giving observed rate constants at a wide range of temperatures in a single run. An advantage of the RPKA/TSR approach is that information may be rapidly obtained even in earliest studies even before a mechanistic framework has been established and requires little mathematical prowess and no specialized computer programs. Continuous temporal analysis may also help inform the study of more complex multi-cycle catalytic networks that are becoming increasingly important in applications including photocatalysis, electrocatalysis, and organocatalytic cascade reactions.