University of Sheffield | Chemical & Biological Engineering

Seminar

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Unravelling Complex Reaction Kinetics for Sustainable Process Development

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Sustainable process development and decarbonization are crucial steps towards the mitigation of climate change and the realization of a more environmentally responsible future. However, facilitating the transition from traditional production methods to the next generation of sustainable processes requires a fundamental understanding of complex reaction systems. Although substantial progress is being made, there are knowledge gaps in unraveling the multiscale chemical interactions of molecules, reaction intermediates, and catalyst active sites. We have developed methodologies for the construction of kinetic models of substantive detail to be built that enable the microscopic atomic scale to be linked with the macroscopic process scale. We have applied our methods to a wide range of different reacting systems, including hydrogenation for fine chemical manufacturing, oligomerization on acidic zeolites, photochemical transformations, and electrolyte thermal decompositions. While these chemistries are seemingly very disparate, applying a common methodology to study them reveals that there are many features of complex reaction networks that are ubiquitous.

This seminar will focus on one of the systems we have examined: the acid-catalyzed conversion of hydrocarbons from renewable sources. We demonstrate that a detailed elucidation of reaction pathways and mechanisms provides the best opportunity for fundamental understanding of heterogeneous acid catalysis, development of more efficient processes, and rational design of novel catalytic systems for improved yields and selectivity of the desired products.