

## CCST Seminar:

- › Friday, April 25, 2008
- › 11:00 A.M.
- › 366 Colburn Laboratory



### Robbie Burch

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Robbie Burch received his Ph.D. in 1968 and his Sc.D. in 1988, both from the Queen's University of Belfast. He is the McClay Chair of Physical Chemistry and head of the School of Chemistry & Chemical Engineering. His research is concerned with developing a fundamental understanding of processes of industrial importance.

#### “Discriminating Between Reaction Intermediates and Spectators Over Water-Gas-Shift Catalysts”

The reactivity of the surface species on ceria-based water-gas-shift catalysts and the corresponding reaction mechanisms have been much debated. The conflicting conclusions are frequently related to the use of extra operando conditions. We report here how a combination of spectroscopic and kinetic data obtained using a single reactor allows discrimination between real reaction intermediates and spectator species. The combined techniques provide a powerful methodology for the investigation of a variety of important gas phase reactions.

A modified version of a commercial reactor was used to obtain kinetic and spectroscopic information under real reaction conditions with good time resolution. The reactivity of the surface species was monitored by DRIFT spectroscopy (DRIFTS) and mass spectrometry (MS) using steady-state isotopic transient kinetic analysis (SSITKA) techniques by switching between reaction mixtures containing  $^{12}\text{CO}$  or  $^{13}\text{CO}$ . The combination of these techniques allowed simultaneous time-resolved monitoring of the variation of the coverage of  $^{12}\text{C}$  and  $^{13}\text{C}$ -containing surface intermediates and the concentration of the gas-phase product  $\text{CO}_2$  due to the isotope exchange. This combined approach, operating under steady-state reaction conditions, has allowed the unambiguous investigation of several potential reaction intermediates and their differentiation from spectator species. The data presented will underline the dangers of using inadequate time resolution or only qualitative information on the amount of reaction intermediates when analyzing possible reaction mechanisms.