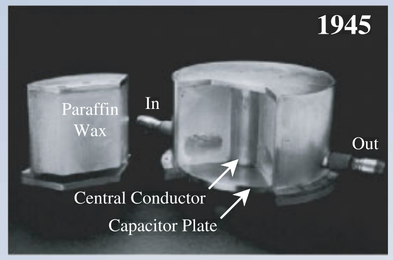
Chemical and Spatial Analyses of Chemical Systems

Toroid Cavity NMR Imagers

PROJECT GOALS

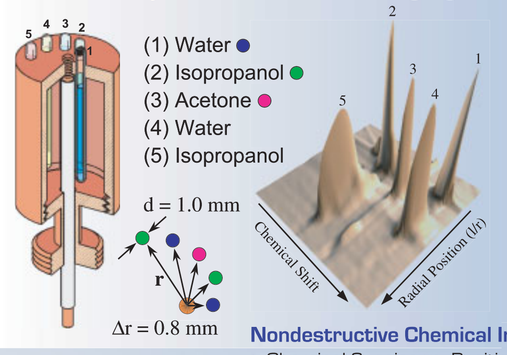
- Address fundamental physicochemical problems in catalysis, radioactive waste, and secondary batteries to advance basic energy technologies.
- Invent and develop detectors for in situ investigations of chemically transforming systems in basic energy technologies.



The toroid cavity detector (TCD) was invented and developed at Argonne to overcome fundamental limitations of NMR detectors in applications to chemical problems in catalysis, nuclear waste, and energy storage.

A Toroid Cavity NMR Imager is a simple, robust, and scalable NMR detector capable of elemental and chemical analyses of materials in the fluid and solid phases with microscopic spatial resolution.

Chemically Selective Radial Imaging



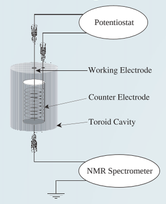
Nondestructive Chemical Imager

- Chemical Species vs. Position (r,θ)
- Quantity/Concentration Profiles
- Mobility and Flow
- Element- and Chemical-Selective

In Situ ELECTROCHEMICAL ANALYSES

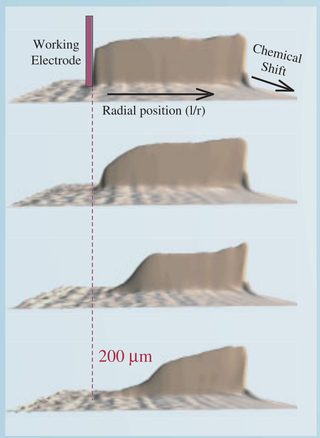
- Transport of cations and anions in novel polymer electrolytes.
- Lithium insertion/extraction in carbon and metal oxide electrodes.
- Architecture and dynamics of oriented molecular film sensors and ion channels.

Near Electrode Imager

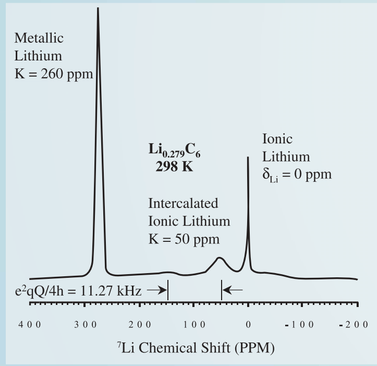


Coin Cell Imager

Ion Concentration Gradient



Lithium Speciation in Li-Ion Batteries



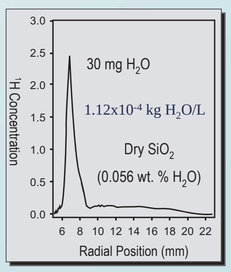
LARGE-SCALE NONDESTRUCTIVE ANALYSES

- Radioactive material stored in sealed metal canisters.
- Composition and flow of processed materials.

Large Scale Samples

Quantitative Analyses

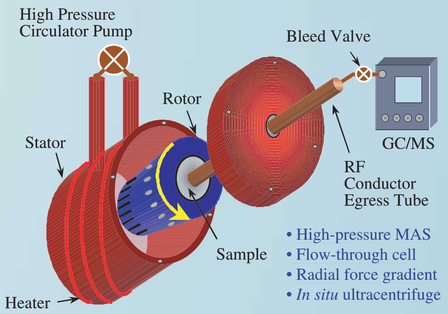
- Sample phase: solid, liquid, gas
- Sample size: 1mg-100 g
- Experiment time: 1min.-10 hr.
- Sensitivity: ppm for ^{1}H



CHEMICAL AND PHYSICAL ANALYSES UNDER EXTREME CONDITIONS

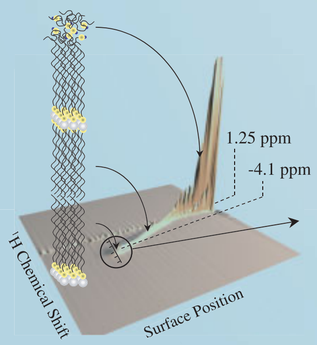
- Homogeneous catalysis in supercritical CO_2.
- Reaction product cross sections in catalyst beds.
- Rheology of stressed soft matter.
- *In situ* ultracentrifuge separations.

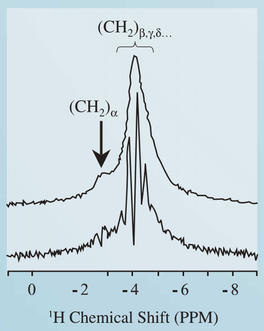
High Resolution Imager for Solids

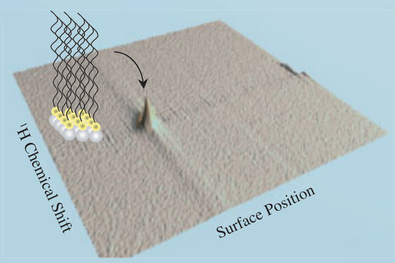


- High-pressure MAS
- Flow-through cell
- Radial force gradient
- *In situ* ultracentrifuge

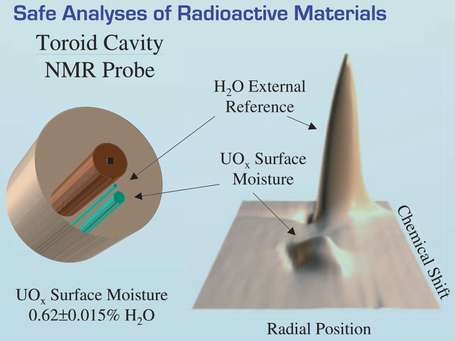
Thin Film Sensors





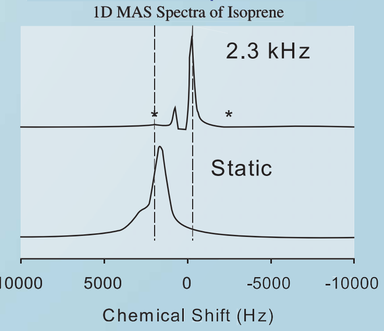


Safe Analyses of Radioactive Materials



Rubber Under Compression Force

1D MAS Spectra of Isoprene



FUTURE DIRECTIONS

- Continue WFO project with WP-AFB on charge transport mechanisms in solid state electrolytes.
- Expand WFO project with Kraft on integrating TCD technology in process streams.
- Continue investigations of the architecture and dynamics of SAMs at the University of Chicago.