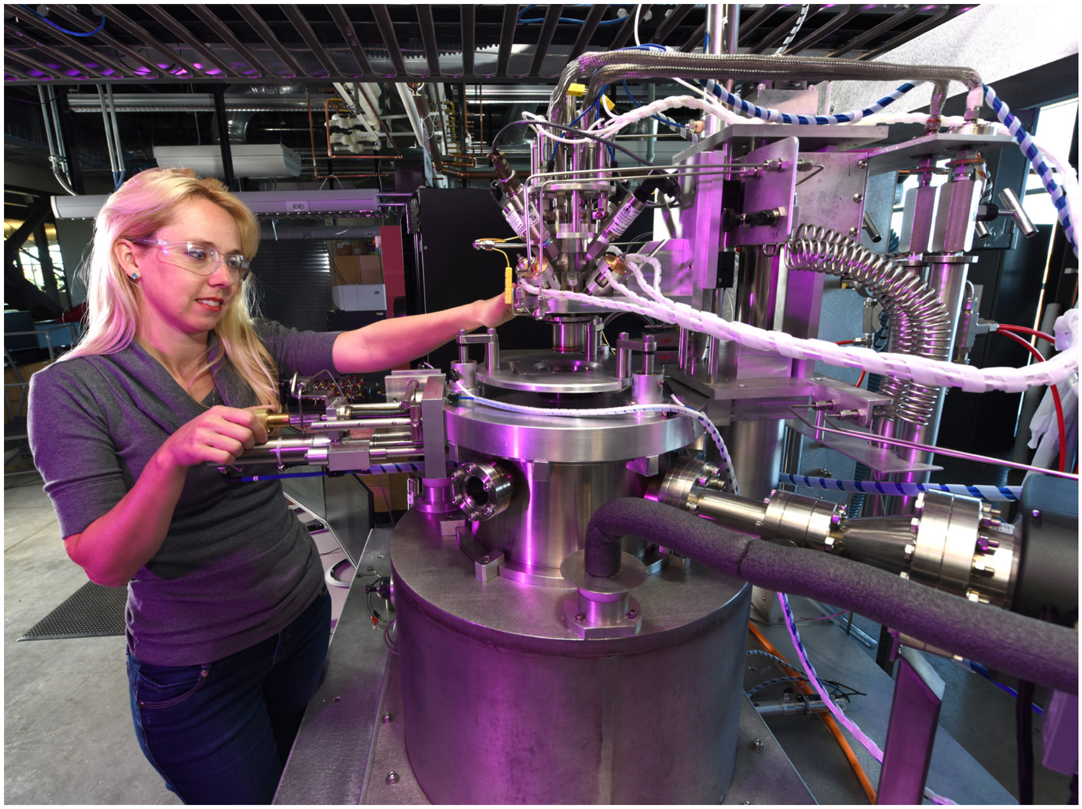


Researchers at Idaho National Laboratory are using a cutting-edge Temporal Analysis of Products (TAP) reactor system to design advanced catalytic materials that use far less energy and minimize waste production.

Changing the World's Energy Future

Idaho National Laboratory

Temporal Analysis of Products

Reactor system for catalyst development

Chemicals are ubiquitous in our everyday lives and are the cornerstone for many of the goods and products purchased by modern-day consumers – everything from diapers to diesel fuel.

But the conventional processes used to make these chemical building blocks are enormously energy-intensive and can result in hard-to-treat waste streams. All of which increases the cost of doing business.

Researchers at Idaho National Laboratory are using a cutting-edge Temporal Analysis of Products (TAP) reactor system to design advanced catalytic materials that consume far less energy while minimizing byproducts and waste streams.

With the TAP reactor, researchers can examine individual reaction steps of a complex catalytic mechanism on a complex catalytic surface. This information enables INL experts to optimize or design multicomponent industrial materials to deliver a specific product or chemical.

What is a TAP Reactor?

The TAP reactor system provides a totally different way of looking at catalysis and materials science problems. It does this by using a probe molecule pulse response to analyze complex reaction kinetics. Fewer than 20 TAP systems exist in the world, and only three reside in the U.S., including two at INL.

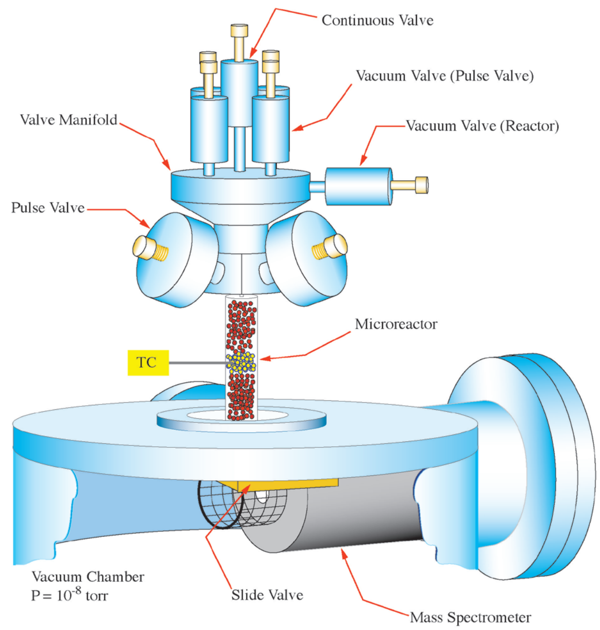
Why the TAP Reactor?

TAP tackles the most challenging catalysis and material science challenges by providing a precise methodology for evaluating complex industrial materials (direct from an operating environment) with a detailed intrinsic kinetic characterization of individual reaction steps.

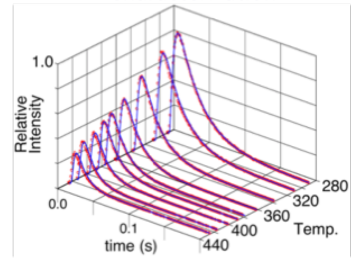
Why Partner with INL?

In addition to having the only TAP "user program" in the country, INL has world-class TAP expertise for solving real-world problems and scale-up challenges, with commercial success as the goal.

The TAP reactor system is located in the Center for Advanced Energy Studies, a



Schematic of the TAP reactor system.



Sample data obtained from a TAP experiment.

public research facility that can be accessed by researchers at other national laboratories, academia and industry.

A Unique Characterization Tool

The TAP reactor system is designed to study the kinetics of gas-solid interactions on complex materials directly from an operating environment. Characterizing the relationship between surface composition and kinetic properties enables the rational design of high-performance materials based on microkinetic detail from simple reaction steps.

The advantage of TAP comes from the small pulse size (approximately 10 nmols), which is several orders of magnitude smaller than the number of active sites in a typical sample. As a result, from pulse to pulse, the kinetic state of the material can be probed without inducing a significant change. Over a long series of pulses, a material can be incrementally manipulated, for example from oxidized to reduced.

Observing the evolution of kinetic properties from TAP data can reveal how "hidden" processes such as bulk oxide transport, surface diffusion, site blockage, reaction products and surface intermediates impact the reaction mechanism. This information can be used to better understand deactivation mechanisms or to distinguish why materials of similar composition and preparation perform differently at process conditions.

How TAP Works

In a typical TAP experiment, a thin zone of active material is tested in a packed bed microreactor under vacuum conditions. A pulse valve injects an ultralow intensity pulse of probe molecules, and the exit flow is detected with a mass spectrometer. Details of the gas/solid kinetic interaction can be extracted from the time-delay characteristics of the reactants and products. A slide valve at the reactor exit allows high-pressure flow experiments for sample pretreatment or conventional reaction studies.

Operating Conditions

The TAP system can accommodate a range of pressure regimes, temperatures and sample forms.

- Pressure: Vacuum pulse response to atmospheric pressure flow
- Temperature: 25 C to 1000 C
- Sample forms: Powders, particles, wire, foils, single crystals, monoliths

Distinguishing Features

Compared to other kinetic techniques, TAP offers:

- Well-defined transport
- Millisecond time resolution
- Negligible mass transfer limitations
- Gas phase uniformity
- Measurement of intraparticle transport in nanostructured materials
- Isothermal operation, even for highly exothermic reactions
- Minimal surface reconstruction
- Time-resolved injection of reactants (pump/probe experiments)
- Incremental composition titration (e.g., manipulation of oxygen content)

For more information

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