Pacific Northwest
NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

Frontiers in Catalysis Science and Engineering
Seminar Series

High-throughput experimentation in combination with statistical methods and machine learning: From structure-property relationships to the discovery of new catalyst

Jochen Lauterbach
Professor
Chemical Engineering
University of South Carolina
Columbia, SC

August 21
10:00 am
EMSL 1077

The development of high-throughput experimentation (HTE) over the past two decades allows researchers to screen large compositional and operational spaces more efficiently, while advances in statistical methods and machine learning (ML) have enabled researchers to systematically explore relationships between synthesis variables, structural properties, and catalytic performance in these HTE datasets.

The first example will discuss a statistical design and analysis that was used to develop cobalt-based oxidation catalysts prepared via one pot metal salt reduction. Emphasis was placed upon understanding the effects of synthesis conditions on the resulting nanomaterial properties. HTE was employed to study the catalytic performance of Co oxidation catalysts over a wide range of synthesis and reaction conditions using a 16-channel fixed bed reactor equipped with a parallel infrared imaging system. Specifically, Co_3O_4 nanomaterials of varying properties were evaluated for their performance as oxidation catalysts. Figure-of-merits including light-off temperature, apparent activation energy, and catalyst stability were measured and mapped back to the catalyst properties and synthesis conditions. Statistical analysis methods were used to elucidate property-activity relationships as well as the design rules relevant for the synthesis of active catalysts.

In the second example, the discovery of novel NH_3 decomposition catalysts will be presented. The first step was to use HTE to screen a limited amount of catalyst compositions and use that training dataset as input to a random forest ML model. The ML model was able to predict new materials, which were subsequently tested, and led to the discovery of two new, highly active catalyst compositions. Advantages and disadvantages of ML as applied to catalyst discovery will be discussed.

U.S. DEPARTMENT OF ENERGY

Host: Zdenek Dohnalek
POC: Diane Stephens

www.pnnl.gov