CHEMICAL CALCULUS: A NEW PARADIGM OF CHEMICAL KINETCS

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Understanding the complexity of chemical reactions in heterogeneous media is an inroad to creating new solid active materials, such as catalysts. Our research focuses on non-steady-state studies and challenges the traditional methods of high-throughput screening of catalytic systems under steady-state conditions.

In my lecture, I will introduce the Temporal Analysis of Products (TAP), an experimental method which has been proposed by Gleaves (1988) and Gleaves and Yablonsky (1997), and Thin-Zone-TAP-reactor (TZTR). Our recent work on further development of the theoretical framework underlying these methods will also be presented. Briefly, in the TAP-approach, systematic small stepwise changes in catalyst surface composition are combined with precise kinetic characterization after each change, to elucidate the evolution of catalyst properties and provide information on the relationship between surface composition and kinetic properties. The TZTR-experiments provide the non-steady-state concentration, transformation rate and uptakes/releases in the active catalytic zone. Then, the new theory (so-called Y-procedure) is used to determine the number of active sites and kinetic parameters of active materials without any *a priori* assumption about the type of kinetic dependence. Finally, the detailed mechanism of a complex catalytic reaction may be revealed. These approaches will be illustrated by examples related to reactions of complete and partial oxidation, and decomposition of ammonia.

Ideas of Chemical Calculus which will be described in detail can be expanded into many different areas and systems, *e.g.* for design of sensors, semiconductors and drugs.

Literature
Books

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