When Two Eyes are Still Better than One: Model Construction vs Model Reduction

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Two complementary strategies in design of rational models of complex catalytic processes, model construction and model reduction, are described and compared. Model construction is performed via the ‘chemical calculus’ approach which is mostly based on the data of the advanced Temporal Analysis of Products (TAP)-method. The experimental information is characterized by

(1) Insignificant change of the active material during a single-pulse experiment and controlled change during a series of pulses
(2) Well-defined diffusion transport taken as a “measuring stick”
(3) Uniformity of the chemical composition across the active zone

The ‘chemical calculus’ approach includes a battery of algorithms, in particular the algorithm for 'kinetically model free' reconstruction of different variables of complex chemical system, reaction rates, gas and surface concentrations. It is shown that real modeling combines both model construction and model reduction. The novel strategy for elucidating catalytic mechanisms of optimal complexity utilizes a concept of kinetic coherency. For model discrimination, the decision tree procedures and patterns of kinetic behaviour are used. Theoretical results are illustrated by examples taken from the catalytic reactions of complete and partial oxidation.

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