326a Challenges in the Field of Catalysis – Implications for Chemical Reaction Engineering

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The ultimate goal of chemical reaction engineering is to predict the performance of a reactor, most often containing a catalyst, based upon the minimum amount of experimental information. If this goal could be satisfied, then it would be possible, in principle, to design a chemical reactor knowing only the size and internal configuration of the reactor, the size, shape, and chemical composition of the catalyst, and the overall stoichiometries of the desired chemical reactions. The past 50 years have been witnessed impressive progress towards this ultimate objective, particularly concerning the design of the chemical reactor once the kinetics of the various chemical reactions occurring in the reactor have been specified. While progress has also been made towards understanding the mechanism and kinetics of catalyzed process from a fundamental level, the advances in this domain are still insufficient to allow for the prediction of catalyst performance (viz., activity, selectivity, and stability) based on first principles, or even empirical based design principles. This talk will attempt to identify some of the challenges for making progress towards the goal of being able to "design" catalysts. A series of examples will be presented to illustrate how progress can be made towards understanding the fundamental issues controlling the relationships between catalyst composition and structure, and catalyst performance.