Joint kinetics: New relationships between thermodynamic and kinetic characteristics (CATL15)

Abstract

New results regarding relationships between thermodynamic and kinetic characteristics create a new situation in chemical kinetics, in heterogeneous catalysis particularly. Joint kinetics is defined as an analysis of a special combinations of kinetic mechanisms and events (intersections and coincidences). A map of kinetic events is constructed and analyzed. A previous dogma ‘it is impossible to predict kinetic behavior based on known thermodynamic characteristics’ has to be corrected. In some cases, knowing the thermodynamic characteristics and kinetic dependencies which start from some initial conditions, it is possible to predict kinetic behavior from other initial conditions. This statement is illustrated by examples taken from heterogeneous catalysis (model examples and the water-gas shift reaction).

New phenomena are analyzed: a momentary equilibrium in the TAP-studies of reversible adsorption; critical simplification in CO oxidation over platinum and ‘counter- equilibrium for the water-gas shift reaction in counter flow diffusion flames. The switching point between thermodynamic and kinetic control in organic reactions is analyzed as well.

References