Microkinetic Model Construction as a Route towards a Better Understanding of Chemical Processes

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Kinetic models can significantly differ in level of complexity, ranging from power laws that merely describe the feed conversion to microkinetic models accounting for all elementary steps in the reaction mechanism. While the former type of models can readily be validated against a limited experimental dataset, the construction of microkinetic ones requires a much more pronounced effort. They come, however, with the advantage of more trustworthy extrapolations beyond the range of experimental conditions against which they were trained. Apart from the microkinetic model by itself, the fundamental insights acquired during its construction may even represent the most valuable asset.

How should such microkinetic models be constructed? Are clear procedures available to follow, result in a guaranteed, adequate model? A literature analysis indicates that a myriad of techniques potentially contributes towards microkinetic model construction. These techniques are classified into 4 main categories, i.e., *surface science* covering experimental techniques yielding specific and detailed information about (a detailed aspect of) the reaction mechanism, *computational chemistry* based on ab initio techniques to determine possible reaction routes and corresponding parameter values, *assumed values* or alternative techniques to those contained in the previous category to determine, a priori, model parameter values, and, finally, *regression* or the adjustment of remaining model parameters such that a best fit is obtained between model simulations and experimental data.

The use of particular techniques belonging to the various categories depends on several factors, the investigated reaction being an important one, as well as the ‘school’ the modeler belongs to and the experience already acquired. It renders an artistic component to microkinetic modeling, which is both a curse and a blessing, as will be demonstrated for example reactions such aromatic hydrogenation, Fischer Tropsch Synthesis and hydrocracking.