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Editorial

Multiscale and Innovative Kinetic Approaches in Heterogeneous Catalysis

Yves Schuurman ¹ and Pascal Granger ^{2,*}

¹ Institut de Recherches sur la Catalyse et l'Environnement, Ircelyon UMR 5256, Université Claude Bernard Lyon 1, 2 Avenue Albert Einstein, 69626 Villeurbanne CEDEX, France; yves.schuurman@ircelyon.univ-lyon1.fr

² Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181—UCCS—Unité de Catalyse et Chimie du Solide, F-59000 Lille, France

* Correspondence: pascal.granger@univ-lille.fr; Tel.: +33-320-434-938

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Kinetics and reactor modeling for heterogeneous catalytic reactions are prominent tools for investigating, and understanding, the catalyst functionalities at nanoscale, and related rates of complex reaction networks. Prominent developments were achieved in the past three decades from steady-state to unsteady state kinetic approaches facing important issues related to the transformation of more complex feedstocks using a wide variety of reactor designs, including continuous flow reactors, fluidized reactors, recirculating solid reactors, pulse reactors, Temporal Analysis of Product (TAP) reactors with sometimes a strong gap in the operating conditions from ultra-high-vacuum to high pressure conditions. In conjunction, new methodologies have emerged giving rise to more sophisticated mathematical models, including the intrinsic reaction kinetics and the dynamics of the reactors and spanning a large range of length and time scales, from the nanoscale of the active site to the reactor scale. Recently, the development of steady-state isotopic transient kinetic analysis coupled with in situ and in operando techniques is aimed at gaining more insight into reactive intermediates.

The objective of this special issue is to provide diverse contributions that can illustrate recent advances and new methodologies for elucidating the kinetics of heterogeneous reactions and the necessary multiscale approaches for optimizing the reactor design.

Among the different contributions provided in this special issue, two articles review and summarize the use of elegant methodologies. In the frame of microkinetic approaches for catalytic reactions, the isolation of the real intermediates among various adsorbates and the calculation of more accurate kinetic and thermodynamic parameters to refine kinetic models are still challenging. In this context, the development of new analytical tools, such as adsorption equilibrium infrared spectroscopy, provides an alternative to classical surface science studies—offering the opportunity to get more accurate heat of adsorptions of co-adsorbed species, and taking the coverage dependency into account in more realistic operating conditions [1]. In general, the extrapolation of kinetic models in very different operating conditions than those applied for its development must be taken with caution leading to unrealistic deviations and over interpretations. In practice, microkinetics cannot be sufficient to get a proper description of complexity, as mentioned by Standl and Hinrichsen [2], who proposed both lumped and microkinetic approaches in catalytic olefin cracking and methanol-to-olefin over zeolites. Useful general and specific recommendations for future modeling of complex networks are given by these authors.

Full papers also proved the usefulness of kinetic approaches especially in the context of an energy transition. By way of illustration, Song [3] paid attention to dehydration of 2,3-butanediol to 1,3-butadiene and methyl ethyl ketone produced from various biomasses instead of fossil resources. It was found that 1D reactor modelling taking into account interfacial and intra particles gradients

can provide important information for further development of commercial processes. Nowadays, computer-aided design can be essential for the prediction of reactor performances. At the macroscopic scale, the use of empirical rate equations is not rigorous and precise enough to fit boundary conditions whereas microkinetic approaches should in principle provide more robust models, but sophistication is usually synonymous with time-consuming. Gossler et al. [4] developed a relevant methodology for reactor simulation for gaining time. It is worthwhile to note that these complex approaches coexist with more conventional approaches performed in the kinetic regime. Such studies can be useful to get more relevant structure-reactivity relationship taking uniformity in the gas phase and the catalyst bed composition as shown by Urmès et al. [5], who concluded that the selective hydrogenation of acetylene on supported palladium-based catalyst involves a single active site. Temporal analysis of products is able to investigate the catalyst behavior in wide conversion range, especially at high conversion generally encountered in more realistic conditions. Because transport regimes can be modeled, those transient experiments can provide the time response of a surface exposed to ammonia, and distinguish between the ability of cobalt and iron to store a mixture of hydrogenated ad-species or predominantly N or NH [6]. Finally, two contributions report lab-scale experiments on structured catalysts, e.g., dense filamentous graphite [7,8], and illustrating the best practice at lab-scale through the comparison of catalysts in powder and tableted form to examine the impact of internal diffusion limitation on the determination of kinetic parameters.

Conflicts of Interest: The authors declare no conflict of interest

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