# Extent-based Model Identification of Surface Catalytic Reaction Systems

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Identification of kinetic models and estimation of reaction and mass-transfer parameters is an important task for monitoring, control and optimization of industrial processes. A methodology called *Extent-based Model Identification* has been developed to separate the effects of reaction, mass transfer, and inlet and outlet flows for homogeneous and gas-liquid reaction systems. The decoupled effects, called extents, are used to decompose the model identification task incrementally into sub-problems of lower complexity, in which measured data are first transformed into extents and these extents are then modeled individually [1-3].

For the analysis of surface catalytic reaction systems, it is important to separate the coupled effects of transport phenomena and reactions. Therefore, the methodology of Extent-based Model Identification has been extended to heterogeneous reaction systems (gas-solid and gas-liquid-solid systems) involving catalytic processes at the surface of a solid catalyst, described by Langmuir-Hinshelwood types of kinetic models.

From measurements in fluid and solid phases, the extent of each individual dynamic process is computed. A model is postulated for that process and the corresponding extent is simulated and compared with the computed extent. This procedure allows separate model identification and parameter estimation for the diffusion of substrates and products, adsorption of substrates, desorption of products and solid-phase reactions.

[1] Bhatt et al., Ind. & Eng. Chem. Res., **2011**, 50, 12960-12974
[2] Srinivasan et al., Chem. Eng. J., **2012**, 208, 785-793
[3] Billeter et al., Anal. Chim. Acta, **2013**, 767, 21-34