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Incremental Model Identification of Gas-Liquid Reaction Systems with Unsteady-State Diffusion

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Identification of kinetic models and estimation of reaction and mass-transfer parameters can be performed using the extent-based identification method, whereby each chemical/physical process is handled separately [1-3]. This method is used here to analyze gas-liquid systems under unsteady-state mass transfer. Such a situation is common in the case of diffusion-controlled reactions and is modeled by the film theory, that is, transferring species accumulate in a liquid film. In both the gas and liquid bulks, mass-balance relations describe the species dynamics as ordinary differential equations (ODE) and serve as boundary conditions for the film. On the other hand, the dynamic accumulation in the film is described by Fick's second law. The resulting partial differential equation (PDE) system is solved by discretization and rearrangement in ODEs.

The estimation of diffusion coefficients follows a two-steps procedure. First, the extents of mass transfer are computed from measurements in the two bulks. Diffusion coefficients are then estimated individually by fitting each extent of mass transfer to the extent obtained by solving the corresponding PDE. Comparison of the estimated diffusion coefficients with their literature values serves to validate the models identified in the two bulks.

The estimation of both kinetic parameters and diffusion coefficients is investigated for gas-liquid reaction systems with unsteady-state diffusion. The approach is illustrated with simulated examples.

[1] Bhatt et al, Ind. & Eng. Chem. Res. 50, 12960-12974, **2011**

[2] Srinivasan et al, Chem. Eng. J. 208, 785-793, **2012**

[3] Billeter et al, Anal. Chim. Acta 767, 21-34, **2013**