REACTION PROGRESS KINETIC ANALYSIS BY DIRECT ANALYSIS OF CONCENTRATION-TIME PROFILES

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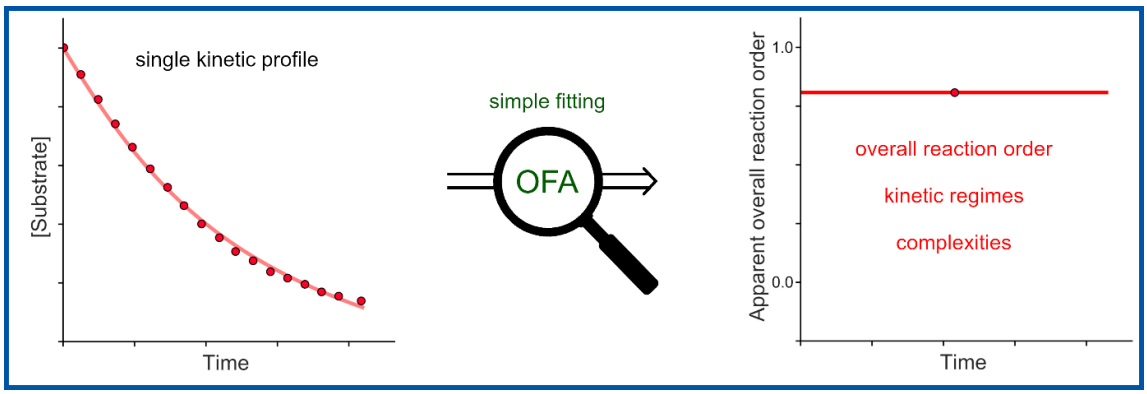
The rapid development of analytical methods have rendered reaction-monitoring to obtain kinetic data a routine step in the development of new chemical reactions and the study of reaction mechanisms. However, analysis and interpretation of kinetic profiles have not enjoyed a parallel development. Only in recent years, with the advent of the Reaction Progress Kinetic Analysis (RPKA) model, introduced by Blackmond, the systematic use of the wealth of information available from kinetic profiles has become commonplace [1]. Recently, Burés furthered the approach by introducing Time Normalization Analysis (TNA) [2,3], which utilizes concentration-time data directly, instead of rate-time data, to determine partial reaction orders of reactions. However, still not all the information contained in kinetic profiles is utilized. Additionally, most of the current analysis methods are not suitable for automatic analysis required for high-throughput experimentation in machine-driven laboratories as they require significant human intervention. Herein, we report on a new general method, which we term Order Fitting Analysis (OFA), to analyze full concentration-time profiles of chemical reactions and extract information regarding the reaction order with respect to substrates, the presence of multiple kinetic regimes, and the presence of kinetic complexities, such as catalyst deactivation, product inhibition, and substrate decomposition. Being in its essence a simple nonlinear fitting approach, it has the potential to be straightforwardly implemented in automated high-throughput kinetic analysis procedures.



[1] Blackmond, D. G. *Angew. Chemie - Int. Ed.* **2005,** *44*, 4302–4320.

[2] Burés, J. *Angew. Chemie - Int. Ed.* **2016**, *55*, 2028–2031.

[3] Burés, J. *Angew. Chemie Int. Ed.* **2016**, *55*, 1–5.