Past, Present and Future of Kinetic Analysis

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Understanding the molecular mechanisms of synthetic transformations remains one of the central challenges in catalysis and is essential for developing more efficient and robust processes. Kinetic analysis provides some of the most valuable mechanistic evidence, and reaction orders are among its most fundamental and informative outputs. This talk will examine the past, present and future of kinetic analysis.

The first part will revisit classical kinetic methods, which developed in response to the experimental technology available at the time. When collecting concentration–time data was laborious, chemists designed methods that relied on a limited number of measurements, such as initial-rate analysis. We will examine the limitations of these classical approaches and highlight their most common experimental and interpretative pitfalls, particularly when determining and interpreting reaction orders.[1]

The present landscape is defined by advances in reaction monitoring. Collecting many data points throughout a reaction has become relatively straightforward, whereas preparing and performing independent reactions remains experimentally demanding. Reaction Progress Kinetic Analysis (RPKA)[2,3] and subsequent visual kinetic approaches, including time-shift analysis,[4] time normalization analysis (TNA)[5] and variable time normalization analysis (VTNA)[6,7], emerged in response to this shift. Instead of reducing each experiment to a single initial-rate point, these methods compare the many points contained within complete reaction profiles. They therefore maximise the number of comparisons that can be made between experiments and extract kinetic information across a broad range of concentrations and conversions from only a few strategically designed reactions.

Finally, the continuing increase in computational power and the current revolution in machine learning[8] are opening a new stage in the evolution of kinetic analysis. These developments may help us analyse increasingly complex kinetic datasets, distinguish between competing mechanistic hypotheses and design experiments that provide the greatest amount of mechanistic information. We will explore these emerging possibilities and consider how they may shape the future of kinetic analysis.

References

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