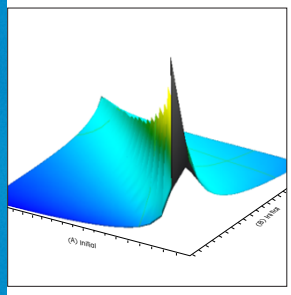
Intelligent Software

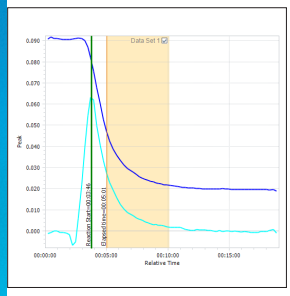
A Faster Way to Optimize Chemistry

Better Insight, Fewer Experiments



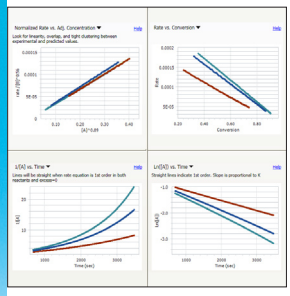
Faster Reaction Optimization

By running a small number of carefully designed experiments, iC Kinetics™ helps chemists and chemical engineers working in Process R&D optimize chemical reactions. The software rapidly develops a kinetic model for the user, then simulates the effect of various starting conditions on the reaction, leading to faster reaction optimization in fewer experiments.



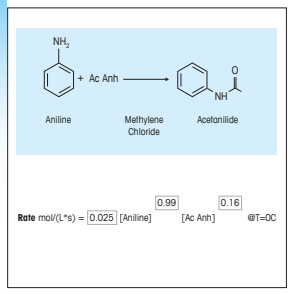
Process Robustness

Understanding how reaction dynamics change during the course of a reaction, especially at the end when conversion is high, is an important aspect of developing a robust process. iC Kinetics™ enables the user to better understand where potential side reactions may occur, helping to predict the onset of undesired reactions leading to by-product formation.



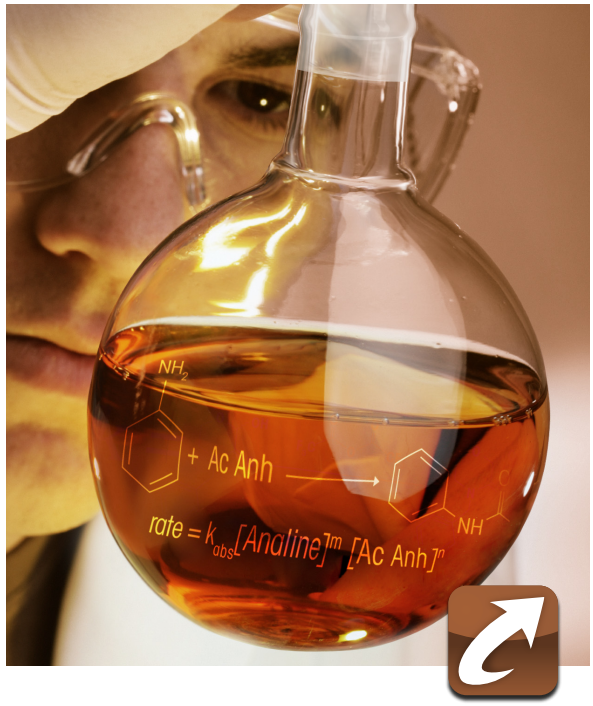
Catalyst Performance

Determining catalyst performance during the course of a reaction is essential to reaction optimization. iC Kinetics™ delivers a graphical method of understanding what actually happens to the catalyst during a reaction, answering critical questions over catalyst stability, poisoning, substrate/product inhibition and impurity formation.



Driving Force Analysis

Driving Force Analysis aids the understanding of safe operational parameters for a given reaction. iC Kinetics™ provides a rapid and comprehensive understanding of these concentration driving forces at the beginning instead of at the end of a mechanistic investigation.



iC Kinetics™ Software

The study of chemical kinetics investigates the influence of various experimental parameters on the rate of a chemical reaction, and gives information which helps the understanding of the reaction mechanism. iC Kinetics™ provides a fast, graphical way to describe the characteristics of a chemical reaction and optimize chemistry. The kinetic model created by the software can be used to simulate the effect of concentration and temperature parameters on the performance of the reaction. This data is generated in fewer experiments than using a traditional approach, leading to a faster way to understand and optimize your chemistry.

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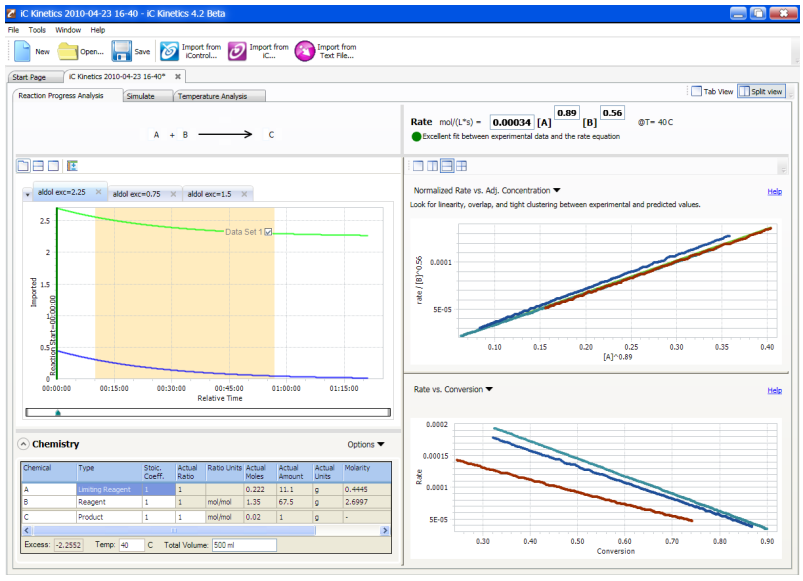
iC Kinetics™ is a simple, graphical method of analyzing how different experimental conditions can influence the speed of a chemical reaction. iC Kinetics™ can seamlessly import concentration data from *in situ* spectroscopic measurements or conversion data from reaction calorimetry for kinetic analysis.

Reaction Progress Data
In order to get maximum information for iC Kinetics™, an accurate means of continuous monitoring of reaction progress is necessary. The reaction data are acquired over the course of a reaction under synthetically relevant concentrations where the concentrations of both reactants are changing simultaneously.

Experimental Design
Reaction conditions are carefully designed to create the same and different excess experiments. Excess is defined as the difference between the starting concentrations of two reactants. The different excess experiments calculates kinetic rate equation while the same excess experiment allows us to understand catalyst performance.

Temperature Dependent Models
iC Kinetics™ is designed to calculate Arrhenius equation for temperature dependent study. As a prerequisite, it also provides capabilities to study any concentration dependency at different temperature. A change in the observed activation energy as a function of similar concentrations with temperature indicates a shift in the controlling mechanism of reactions.

Simulate and Optimize
Using the rate equation or Arrhenius equation, iC Kinetics can simulate hundreds of experiments to create an interactive 3D surface plot for optimum conversion calculation. By clicking on surface plot, iC Kinetics™ will calculate the optimum starting concentrations and display reactants and product profiles in a trend window.



PC Specifications (Minimum Requirements)

	Single iC Application	Multiple iC Applications
Operating System	Windows XP™ SP3 or Vista SP1 or Windows 7	Windows XP™ SP3 or Vista SP1 or Windows 7
CPU	Intel Core 2 Duo 2.2 GHz T7500 (Notebook) or 2.4 GHz E4600 (Desktop)	Intel Core 2 Duo 2.5 GHz T9300 (Notebook) or 2.8 GHz E8300 (Desktop)
Memory	2+ GB RAM or more	3 GB RAM or more
Hard Disk	SATA 5400 rpm	SATA 7200 rpm
Graphics	SXGA 1280x1024 with 3D hardware acceleration, including Vertex Shader, Pixel Shader, Texture Support, and Lighting	SXGA 1280x1024 with 3D hardware acceleration, including Vertex Shader, Pixel Shader, Texture Support, and Lighting
Additional Software	Internet Explorer 7.0 Microsoft Office 2003 or 2007	Internet Explorer 7.0 Microsoft Office 2003 or 2007

Accelarate Development with iC Suite
The iC Suite of software products support METTLER TOLEDO *in situ* spectroscopy, particle system characterization, precise reactor and calorimetry. iC software integrates your entire experimental workflow making it simple to visualize, interpret and report your results.

- **Intuitive, Consistent User Interface**
- **Seamless Integration Between Products**
- **Easily Transform Data into Information**

To learn more visit **www.mt.com/iC**

References

1. Blackmond, D. G., Angew. Chemie Int. Ed., 2005, 44, 4302
2. Blackmond, D. G., et al., J. Org. Chem. 2006, 71, 4711

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