Intelligent Software

iC Kinetics™ 5.0
Release Notes

Dear Customer,

Thank you for purchasing iC Kinetics™ 5.0, the simply powerful and intelligent software package to understand and optimize chemistry. Everything you need to install and run iC Kinetics™ 5.0 is stored on the installation media (CD-ROM or downloaded zip file).

Contents of the Installation Media

- iC Kinetics™ 5.0 software installer (AutoRun.exe)
- iC Kinetics™ 5.0 Release Notes (this file)
- iC Kinetics™ 5.0 Installation Guide
- iC Kinetics™ 5.0 Documentation Portfolio

For optimal viewing of the Installation Guide and Documentation Portfolio, use Version 9 of Adobe Acrobat Reader.

Installation Guide and System Requirements

Please install iC Kinetics™ 5.0 according to the installation guide which can be found on the installation media. This also describes the minimum PC requirements to install and run iC Kinetics™ 5.0.

User Guide and Help File

The iC Kinetics™ 5.0 Help file is available from the software and can be printed by the user from the included User Guide PDF. To access the context-sensitive Help from a specific place in the software, click in the software window and then click F1 on your keyboard.

Customer Support

If you encounter any issues with iC Kinetics™ 5.0, please don't hesitate to contact your sales representative or service engineer, or contact us at:

iC@mt.com for Software Support

METTLER TOLEDO

Issues Addressed in Service Pack – Version 5.0 SP1

Enable Compatibility with New iControl™ 5.1 and 5.2

The newer iControl™ 5.1 and 5.2 versions included some changes to the chemical table and data sharing protocols that caused issues with importing data into iC Kinetics™. This issue has been resolved in the service pack.

Features for Version 5.0

Full Support for Windows 7 and Vista Operating Systems

iC Kinetics™ 5.0 fully supports the 32-bit and 64-bit versions of Windows Vista and Windows 7 as well as Windows XP.

Extensive Context-Sensitive Help

iC Kinetics™ integrates detailed, context-sensitive help. Pressing F1 while running iC Kinetics™ will display the help file page that is most relevant to the current active window. In each section of iC Kinetics™ document, hyperlinks are also provided which displays the most relevant help information to that section.

Start Page

The main iC Kinetics™ Start Page which appears when the application is started provides easy access to creating or opening iC Kinetics™ documents, helps users to design experiments for reaction progress kinetics analysis, and enables users to create and manage chemicals in chemical database.

Supports Importing Trends from Other iC Software

Any experiment from an iC application (iC IR™, iControl™, iC FBRM™, etc.) can be imported into iC Kinetics™. The iC application does not have to be running or installed on the iC Kinetics™ PC. From iC IR™, iC Quant™ trends, ConcIRT™ trends, user defined trends, or peak profiles can be imported for kinetic analysis. Similarly, from iControl™, conversion and temperature trends can be imported. Conversion trends from calorimetry data can be used for kinetic analysis.

Rate Equation

Results from kinetic analysis are displayed as a kinetic rate equation. iC Kinetics™ continuously updates the rate equation as changes are made in the data for kinetic analysis. This makes the impact of any changes immediately apparent.

Chemical Database

A chemical database is installed with iC Kinetics™. This database stores chemical names, physical properties, and structures. Structures can be imported from a standard mol file or can be drawn by the user if ChemDraw version 7.0, 9.0, or 11.0 is installed on the PC.

Note that the chemical database is shared with any iControl™ version 5.0 applications that are also present on the PC.

Reaction Editor

The default chemistry in iC Kinetics™ is A + B -> C. If desired, this default chemistry can be changed to reflect the actual chemistry being investigated by adding chemicals to the reaction editor from the chemical database. Reactant names are then displayed throughout the iC Kinetics™ document for easy visualization.

Chemistry Table

The chemistry table allows users to enter the molar concentrations or amounts for chemicals defined in a reaction. Any chemistry information, such as chemicals and their amounts, defined in an iControl RC1e™ 5.0 experiment is seamlessly imported in iC Kinetics™. iC Kinetics™ will scale absorbance trend to concentration based on starting amounts of each reactant.

Trend Viewer

The Trend Viewer area displays trends from any imported experiments. All of the functionality of the trend viewer from the popular iC software is available in iC Kinetics™. Users can also copy and paste trend from any other iC software products.

Data Sets

The Data Sets are one or more highlighted regions of trends that allow you to select data set regions for kinetic analysis. A data set is a subset of a concentration trend that is used for kinetic analysis.

Reaction Progress Charts

iC Kinetics™ provides Reaction Progress and diagnostics charts that may lead to deeper understanding of the studied reaction. Available charts include – Time Trends charts, Concentration charts, Turnover Frequency charts, Normalized Rate charts, and Integrated Rate Equation charts.

Save Rate Equation

The 'Save Rate Equation' button located at the top of the iC Kinetics™ document also allow the user to save the current rate equation for use in simulation and temperature dependent kinetic models.

Simulation

The 'Simulate' tab on an iC Kinetics™ document allows users to optimize reactions by simulating experiments using a rate equation built from experimental data. iC Kinetics™ calculates the time it takes to reach a conversion value that you specify. The results of the set of experiments are summarized in a 3D plot so the effects of starting conditions on the time it takes to reach the desired conversion can be easily visualized. Selecting a location on the surface plot displays a corresponding 2D trend chart for that simulated experiment.

Temperature Dependent Models

The 'Temperature Analysis' tab of an iC Kinetics™ document displays an Arrhenius plot, calculates activation energy and frequency factor, and displays the temperature dependent rate equation. Study the concentration effect of temperature in Arrhenius plots at various concentrations of the reactants.

One-Click Reporting

One-click reporting is available for an iC Kinetics™ document. The report is a Microsoft Word document that can be edited, saved, and printed by the user.

In addition to generating reports in Microsoft Word, iC Kinetics™ can also report directly to an XPS document. XPS (XML Paper Specification) was developed by Microsoft to provide a read-only definition for document layout and formatting (similar to what an Adobe PDF provides). Users can generate non-editable reports using XPS, and they can also create and view reports even if they do not have Microsoft Word installed on the PC.

Licensing

iC Kinetics™ incorporates a licensing scheme to control the distribution and use of the software. For details on activating the software, please see the iC Kinetics™ Installation Guide.

Software Support

iC Kinetics™ allows users to view system log files, export files to disk and even report issues with the software. The customer support program is part of our commitment to ensure that all system issues are addressed promptly and effectively.

Known Issues

No.	Issue	Description and Workaround
1 31594	**Data Sets Viewer Updating** In the list of data sets, the temperature may not update after the user enters a new value for temperature.	To update the view, uncheck and then check the "Use in calcs" checkbox for each data set.
2	**Molarity Values** If you have molarity trends, and if you have more than 3 reactants, removing one of the reactants, will cause the starting molarity value (shown in the Chemical Table) to be cleared.	Move the reaction start time line in the trend viewer to force iC Kinetics to update the starting molarity fields in the Chemical Table
3 40865	**Actual Moles Cell is Blank** If you enter data to calculate the starting molarity in the iControl import dialog, the starting molarity is correctly calculated, but the Actual Moles field in the Chemical Table is blank.	Move the reaction start time line in the trend viewer to force iC Kinetics to update the Chemical Table. Be aware that the actual amounts are not imported from an iControl experiment, even if you used iControl to do the reagent additions. Molecular weights and stoichiometry however are imported.