Reaction Calorimeter

iControl RC1e™ 5.6
Release Notes

Dear Customer,

Thank you for purchasing iControl RC1e 5.6, the simply powerful software package for the METTLER TOLEDO RC1e Reaction Calorimeter.

Contents of the Installation Package

- iControl RC1e 5.6 Software Installer (setup.exe)
- iControl RC1e 5.6 Release Notes (this file)
- iControl RC1e 5.6 Quick Install Guide
- iControl RC1e 5.6 Installation Guide for Administrators
- iControl Data Conversion Utility for WinRC experiments
- iControl Mixing Guidelines
- iC Data Share Microsoft® Excel® Add-in
- UCB Firmware 3.4.2 for Universal Control Box (UCB) and RTCal Box

Installation Guide and System Requirements

Please install iControl RC1e 5.6 according to the Quick Install Guide. This also describes the minimum PC specifications needed to install and run iControl RC1e.

Tutorial Videos and Help File

We highly recommend watching the Tutorial Videos accessible from the iControl RC1e 5.6 Start Page. These brief videos provide an excellent overview of the software and allow new users to familiarize themselves with iControl in minutes. For more in depth help, a comprehensive Help File is available. To access the context-sensitive Help from a specific place in the software, click in the software window and then press F1 on the keyboard.

Customer Support

If you have any questions or encounter any issues with iControl RC1e 5.6, please contact your local Account Manager or Service Engineer, or contact us at:

Support.RXE@mt.com for General Support on Reaction Engineering

iC@mt.com for Software Support

METTLER TOLEDO

Feature Comparsion Table

Key features of iControl RC1e 5.6 compared with earlier versions of iControl and WinRC:

Feature	WinRC 7.12	iControl RC1e 4.0	iControl RC1e 5.0	iControl RC1e 5.3	iControl RC1e5.6
Easy Data Collection and Instrument Control					
Create your recipe automatically	X	✓	✓	✓	✓
One click on the reactor to change any setpoint	X	✓	✓	✓	✓
iC-iControl: Automatically synchronized reactor data, ReactIR™ data, Raman data, FBRM® data in one experiment, drag and drop of trends	X	✓	✓	✓	✓
Supports Real Time Calorimetry RTCal™	X	✓	✓	✓	✓
Chemistry Table for easy illustration of chemical reaction and chemical amounts in design and analyze mode of experiments	X	X	✓	✓	✓
Improved RTCal calibration and adjustment procedure to increase precision and accuracy of measurement	X	X	✓	✓	✓
Allow reflux factor estimation for RTCal	X	X	✓	✓	✓
Global settings for trends and y-axis. Allows setting defaults for trend view such as displayed trends, color of trends etc.	X	X	✓	✓	✓
New ‘Setpoint by expression mode’ for UCB dosing allows dosing profiles that follow an IR/FBRM signal	X	X	✓	✓	✓
Various extensions for manual dosing such as starting /stopping the operation without user interaction.	X	X	✓	✓	✓
Audible alert for operator message	✓	X	✓	✓	✓
New thermostat mode: Hold actual value (T_r or T_j)	X	X	✓	✓	✓
New ‘Setpoint by expression’ mode for UCB PID controller	X	X	X	✓	✓
U value extrapolated during runtime enabling live values for qr_hf, UA and cpr trends	X	X	X	✓	✓
Manual correction of UA (Besides U)	X	X	X	X	✓
Live Annotation Exchange with connected iC 4.4+ Applications	X	X	X	X	✓
Intuitive Data Analysis and Visualization					
Start Page: One click access to experiments, help file, all hardware manuals, application notes,	X	✓	✓	✓	✓
Compare trends of different experiments in one graph	X	✓	✓	✓	✓
Mixing guidelines	X	✓	✓	✓	✓

Feature	WinRC 7.12	iControl RC1e 4.0	iControl RC1e 5.0	iControl RC1e 5.3	iControl RC1e5.6
Chemical Database	X	✓	✓+	✓+	✓+
Various extensions for chemical database: • grouping of chemicals • new "Comments" field • More straight-forward import/export • Chemical database shared between all iControl versions and iC Kinetics™ on the same PC	X	X	✓	✓	✓
Support for iC Safety™ – An easy to use add-in to assess the thermal risks of your reaction.	X	✓	✓+	✓+	✓+
iC Safety one click evaluation of multiple dosings inside a single integral	X	X	X	✓	✓
Option to use non-averaged calculation for qdos	X	X	✓	✓	✓
Cpi values of UCB sensors considered for calculations	–	X	✓	✓	✓
Option to define if qc is compensated for the qr calculation	X	X	✓	✓	✓
Tr information available in U and cpr tables	X	X	X	✓	✓
'Save as' menu item added allowing to store a copy of the current experiment	X	X	X	✓	✓
Customize tab locations allowing users to see up to 3 different views on one screen.	X	X	X	✓	✓
Short and easy to understand Tutorial Videos explaining how to use advanced features of iControl	X	X	X	✓	✓
Tr, Tj, R, Vr and Mr values for every executed operation or added annotation available	X	X	X	✓	✓
Any offline analytics sample documented in iControl is transferred to iC IR (7.x) and vice versa	X	X	X	X	✓
Quick Reporting and Data Exchange					
One-click Reporting of Results	X	✓	✓	✓+	✓+
Easy and flexible WYSIWYG Report Designer including export to Microsoft® Word®	X	X	X	✓	✓
Multiple Trend Snapshots in Report	X	X	X	✓	✓
Drag and Drop trends from and to Microsoft® Excel® into iControl RC1e	X	✓	✓	✓	✓
Print feature added to more screens to allow printing of individual screen views into an ELNB	X	X	✓	✓	✓
Sensor history report contains adjustment values of all available sensors (Thermostat, RD10, UCB, RTCal)	X	X	✓	✓	✓

Feature	WinRC 7.12	iControl RC1e 4.0	iControl RC1e 5.0	iControl RC1e 5.3	iControl RC1e5.6
Integration with iC Data Share™ for real-time sharing of trends with Microsoft® Excel® and other third party applications.	X	X	X	✓	✓
Support for iC Data Center to automatically capture, prepare and share experiments	X	X	X	✓	✓
Automated site license distribution with iC Data Center	X	X	X	X	✓
Compatibility					
Convertibility of WinRC data into iControl (trends and eval)	–	✓	✓	✓	✓
Microsoft® Windows® XP compatibility	✓	✓	✓	X	X
Microsoft® Windows® Vista compatibility	X	✓	✓	X	X
Microsoft® Windows® 7 compatibility	X	X	✓	✓	✓
Microsoft® Windows® 8.1 compatibility	X	X	X	✓	✓
Microsoft® Windows® 10 compatibility	X	X	X	X	✓
64bit Support for Office version	X	X	✓	✓	✓
64bit Support for Office and Instrument version	X	X	X	✓	✓
Connectivity to iC 4.0 applications or higher	X	✓	✓	✓	✓+

✓ = Supported feature ✓+ = Supported feature with enhancements X = Not supported

These release notes summarize incremental changes in iControl RC1e.

Enhancements for Version 5.6

Manual Entry of UA (Besides U)

Manual corrections or entries in the U table can either be U or UA instead of just U as it was in the previous version. Also the U table has been extended with a UA column.

Annotation Exchange with Connected iC Applications

iC analytical applications with version 4.4 or higher (such as iC PVM 7.0 and iC FBRM 4.4) now support real-time exchange of annotations. If an iControl experiment is linked to an iC experiment (either by being setup in the iControl equipment setup or by including a trend from the other experiment), then any new annotations added in one of the experiments will automatically be added to the other experiment. Note that for this to work correctly, both the iControl experiment and the iC experiment must be open.

Automated License Update through iC Data Center for Site License Users

If connected to iC Data Center, Office licenses and D2I (Data to Information) module options are automatically received from iC Data Center when iControl starts up. There is no longer the need to manually update the site license file for every office PC independently when the site license is renewed. Note that this does mean that users of Office copies should connect their system to iC Data Center under the 'Tools' menu in order to receive these automatic updates.

Offline Analytics Sample Sharing with iC IR 7.x

Every sample taken/documented on the touchscreen or in iControl is automatically transferred into the the new Offline Analytics Sample table in the corresponding iC IR experiment. Once results from offline analytics (e.g. HPLC) are available, they can be easily entered into iC IR and correlated to peak trends.

Support of Windows 10 64-bit Operating Systems Added

iControl RC1e now fully supports Microsoft® Windows® 10 and all 64-bit versions of the Microsoft® Windows® 7 and 8.1 operating systems.

Compatibility Tables

The following table provides an overview on compatibility between iControl RC1e and iC Data Center:

	iC Data Center 5.2	iC Data Center 5.4 / 5.5	iC Data Center 6.0
iControl RC1e 5.0	✘	✘	✘
iControl RC1e 5.3	✓ (with Add-in)	✓	✓
iControl RC1e 5.6	✘	✘	✓

Known Issues

No.	Issue	Description and Workaround
1 FB31725	**RTCal Reminders** Reminders require RTCal adjustment instead of calibration	On systems where iControl 4.0 was previously installed, reminders in iControl 5.6 may request user to perform an RTCal adjustment. Note that the reminder should say "calibration" instead of "adjustment". An RTCal adjustment is only required if a calibration fails.
2 FB19442	**iC Safety: Using WinRC 7.1x or 7.2 Experiments** Calculations related to dosings incorrect for experiments converted from WinRC 7.1x or V7.2	For experiments converted from WinRC 7.1x and 7.2 all heat curves that use the balance trends are incorrect because the balance curves start with the start of the experiment and end with the end of the experiment. **Workaround:** De-activate the automated dosing(s) displayed in the dosing table and add a manual addition with the respective mass, cP, temperature and the correct start and end time.
3 FB576	**Firewall Warning** Appears when starting iControl	On most PCs you will see a firewall warning that iControl is trying to access the network and that this is blocked and needs to be opened by a network administrator. iControl only uses network access for communicating to other iC applications if they are installed on a different PC. For more information on this, please refer to the iControl Installation Guide. If you are not planning to communicate with iC applications over the network, you can simply ignore this firewall warning.
4 FB20844	**Error Loading an Experiment** Conflict due to different RC1e/ RD10 equipment database with different contents	If an experiment in design mode is copied to another computer that has a different equipment database with different content, error messages may appear during the loading of the experiment. These error messages occur because the equipment name and/or respective ID are different. **Workaround:** The experiment can still be loaded, however, the equipment which is missing will not be displayed correctly, and in order to run this experiment, you will need to configure the missing equipment in the experiment equipment setup again.

No.	Issue	Description and Workaround
5 TFS17920 TFS17851	**Migrating Configuration** Some items not migrated from version 4.0/5.0 to version 5.6	The following equipment from older versions is not migrated when installing version 5.6: • Custom insert types • Equipment Setup Templates **Workaround:** Add the equipment manually.
6 TFS17850	**Older iControl 4.0/5.0 Not Working After Installing 5.6** Corrupt iControl 4.0/5.0 equipment database after installing 5.6	After installing version 5.6, the equipment database in older versions needs to be manually upgraded if you still want to work with the older version. The EqDB update can be done as follows: • Go to the Start Page of iControl 4.0/5.0 and click on "Manage Equipment" • Then click on "Update Database"
7 TFS17979	**RD10 Configuration** Configuration Wizard for 2nd and 3rd RD10 Not Working	The wizard to configure new RD10s is not working for RD10 on position 2 and 3. This leads to issues when creating an equipment database from scratch. **Workaround:** Please contact support.rxe@mt.com.
8	UCB pH Control operation is not working properly with the "Hold actual value" task	Option "Add to Mr" for UCB pH Control operation has no effect when using the "Hold actual value" task. **Workaround:** Use the "Ramp by duration" or "Ramp by rate" tasks if you want to track the dosed substance of the pH Control operation in the Mr trend.

Enhancements for Version 5.3

Easy Data Collection and Instrument Control

Live Values for qr_hf, UA and cpr Trends

U values are being extrapolated as soon as a first U value is available. The constant availability of U allows the live calculation of the qr_hf, UA and cpr trends and hence the availability of live heat data. Note that the trend values may change as soon as a new U value gets calculated. In case highly accurate live heat data is required, RTCal technology will provide better data.

New 'Setpoint by expression' Mode for UCB PID Controller

The Control PID Loop operation for the UCB (Universal Control Box) has an additional option that now allows the setpoint to be determined by an expression.

Intuitive Data Analysis and Visualization

New Version of iC Safety

iC Safety is a crucial tool for evaluating the thermal risks of a chemical reaction at industrial scale for use by novice, as well as advanced users. iC Safety summarizes key safety information in an easy-to understand graphical format and provides access to detailed safety data for expert users. In the new 5.3 version, the user interface has been simplified to enable a better user experience for all user levels. In addition, functionality has been added to evaluate multiple dosings or reactions at one time by dragging a single integral over several dosings or reactions.

Tr Information Available in U and cpr Tables

The U and cpr tables contain a new column with the Tr value that was current at the time of the corresponding U or cpr determination.

'Save as' Menu Item Added

Under the 'File' menu, a new item 'Save as' has been added allowing the user to store a copy of the current experiment, including all of its data, at any time.

Tr, Tj, R, Vr and Mr Values for Every Operation and Annotation Available

In the recipe contained in the new report designer, you may show Tr, Tj, R, Vr or Mr values for every operation or annotation. Use the 'Select Columns' icon on the Recipe item to choose which columns to display.

Moving Tabs into Different Screen Areas

In previous versions of iControl, the tabs available for each viewer pane were fixed. For example, it was not possible to see the 'Trends' at the top and the 'Procedure' at the bottom. iControl 5.3 gives you unlimited freedom to move tabs into different screen areas and customize the screen as you prefer it. Simply grab the tab and drag it to the new pane that you wish it to be displayed in. The system will remember the tab locations for each experiment mode (Design, Run, Analyze).

Quick Reporting and Data Exchange

Report Designer Available as Part of Experiment

iControl 5.3 features an easy to use WYSIWYG (what you see is what you get) Report Designer allowing users to create experiment reports that fit company's standards. A new 'Report' tab is included as part of every iControl 5.3 experiment which by default includes all the significant data from an experiment. The user can easily customize this report from within iControl by simply dragging & dropping items such as Trend Graphs or the Experiment Recipe. Users can also add experiment specific text or images from other sources to the report before, during, or after the experiment completes. The resulting report can then be exported to Microsoft® Word® so it can be easily shared with others.

Support for iC Data Center

This version of iControl RC1e supports iC Data Center 5.2. With iC Data Center, all data generated on any supported instrument or software (EasyMax, OptiMax, iC IR, iC FBRM or iControl) is automatically captured and stored in a central file share. A Microsoft® Word® report and Excel® file are then prepared automatically and stored in the same location. The data is shared by sending an email to the user containing a link to the files.

For more information about iC Data Center, visit www.mt.com/icdatacenter.

Integration with iC Data Share Microsoft® Excel® Add-in

The iC Data Share software application is an add-in module for Microsoft® Excel® that allows real-time sharing of data. iC Data Share can pull data from a running iC or iControl experiment into Microsoft® Excel® so that it can be used in calculations, and any resulting values can be sent back to iControl and trended. This provides an easy way to integrate live data from other third party applications that support Microsoft® Excel® interfaces.

The installer for the iC Data Share add-in is provided in a separate folder on the iControl 5.3 Installation DVD or downloaded zip file. iC Data Share can be installed on the same computer as iControl 5.3 or on a different computer as long as it has network access to the iControl system.

Compatibility

Support of Windows 8 and 64-bit Operating Systems Added

iControl RC1e now fully supports Microsoft® Windows® 8/8.1 and all 64-bit versions of the Microsoft® Windows® 7 and 8 operating systems.

Enhancements for Version 5.0

Easy Data Collection and Instrument Control

Chemistry Table

The chemistry table is a completely new integrated feature module that allows the user to easily define the chemical reaction and calculate the amounts required. The chemistry table contains an intelligent calculation engine that is directly linked to the chemical database and that determines the required amounts based on the given stoichiometric factors and ratios. The calculated amounts are directly linked to the dosing table of the experiment.

Improvement of RTCal Calibration and Adjustment Procedure

RTCal is a unique METTLER TOLEDO calorimetry technology which allows an online measurement of heat data without the need for an experiment calibration. In order to achieve the optimal reliability of the measurement it is advisable to have the heat flux sensor bands adjusted by a METTLER TOLEDO field service engineer upon installation of the system and then to calibrate the sensors on a regular basis. The wizard to run the adjustment and calibration were improved extensively so the procedure is as easy and robust as possible.

Reflux Factor Estimation with RTCal License

The operation "HF Qreflux factor determination" has been renamed to "Qreflux factor determination" since this operation is now also available for users with an RTCal license. In previous versions this operation was restricted to users with a Heat Flow license.

New Mathematical Functions for User Defined Trends (UDTs)

Besides the four arithmetic functions (+ - * /), an additional six mathematical operations have been added to UDTs: first derivative, averaging, natural logarithm, logarithm, n^{th} root, and exponentiation.

New Trend for Elapsed Time to Be Shown

A new Elapsed Time trend reflects the time passed since the start of the experiment.

Global Settings for Trends and Y-Axis

The "Save current settings" functionality for the trends tab has been enhanced. It is now possible to define global trend view settings that are applied to every new experiment. The user can define the trends to be shown including the name, color, line width, line style and the settings for the y-axis like the minimum and maximum value, auto scaling, logarithmic and show grid properties etc. These settings are kept persistent and valid for every system user.

Copying User Defined Trend (UDT) During Run-Time

In the previous software version, when copying and pasting a UDT into a running experiment, the UDT immediately became read-only. With the current release the user has the ability to edit a user defined trend when pasting it into a running experiment.

Selectable Unit Check for User Defined Trend

By default the option "Enforce units compatibility" is selected. This means, the editor checks that all terms of the expression have compatible units.

If you select "Ignore units", this check is omitted and the resulting units can be defined manually:

Visibility of Set Value for Mass During Dosing with UCB Equipment

Beneath the end value, the actual mass and the dosing rate, now the set mass is displayed so it is available at first glance on the live equipment picture of the dosing controller.

Visibility of Temperature Control Parameters (P&I)

The T_r control parameters P (Amplification) and I (Reset Time) are now visible during runtime in the tooltip for the reactor. Within the start operation of an experiment the setting of the P parameter can be viewed during runtime and can be adapted to either an organic or an aqueous reaction mass during the design phase of an experiment.

Change of RD10 Dosing Rate During Running Dosing Operation

The dosing rate of a running RD10 dosing loop can be changed on the fly by entering a new value in the equipment overview (same behavior as for UCB dosing controller).

Dosing Profile Based on Arbitrary Expression

It is now possible to perform a dosing task against any available trend or against a user defined trend.

Completion of Manual Dosing without User Interaction

The user can now decide within the Manual Add task whether or not a user interaction or acknowledgement is required to complete the operation.

Play an audible alert during Acknowledge Message

It is now possible to insert an operator message at any point of the procedure that will play an audible alert. This alert can be a custom wave or mp3 file and can be configured to be repeated until the user acknowledges the message.

New Thermostat Mode to Hold Actual T_r or T_j Value

This useful option for the "Heat/Cool" operation will keep the actual temperature value (T_r or T_j mode) constant. This new set temperature is visible in the experiment event log.

Option to Switch Off Overfill Warnings during Whole Experiment

During the setup of the reactor (double click on the reactor in the equipment setup) a new option "Warn if reactor contents exceeds maximal volume" has been added. This option is by default switched on – but can be deactivated by the user.

Intuitive Data Analysis and Visualization

New Version of iC Safety

iC Safety is a crucial tool for evaluating the thermal risks of a chemical reaction at industrial scale for use by novice, as well as advanced users. In addition, iC Safety summarizes key safety information in an easy-to understand graphical format and provides access to detailed safety data for expert users. In its new version 5.3, this D2i (Data to Information) module provides an even more enhanced interface and improved functionality such as the calculation of TD24, criticality classes, analysis of multiple reactions and the ability to take snapshots for the comparison of results. Watch the iC Safety tutorial video for an introduction to this very powerful tool.

Custom Offset for Int(qr_rtc)

The integration of qr_rtc now uses the real baseline. In previous versions the integration was always done from zero.

Basepoint Proportionality Can Be Defined and Kept Persistent

The default basepoint proportionality for cpr, Reflux Factor, U and Vv can now be changed and kept persistent for each experiment and each user within the "Options" window of iControl.

The Points of a Manual Baseline Can Now Be Edited Easily

For a baseline or a baseline with integral it is now possible to select the type "Manual". Using this type makes it possible to add or edit baseline-points using drag-and-drop. Alternatively it is also possible to enter the exact values for changed or added points within a separate window.

Option to Decide if Averaged Dosing Rate (qdos) Should Be Used

During the determination of the terms for qr_hf and qr_rtc, it can be decided if an averaged derivation for the dosing rate (qdos) should be used or not.

The Cpi Values of UCB Sensors Are Considered for Calculations

While setting up a UCB sensor it is now possible to define Cpi values with respect to a specific reactor type. Using the option "Linked to" allows the user to link the selected sensor to the Cpi values

of another sensor already defined in the equipment database. Simply choose the sensor to link to from a dropdown list and the Cpi values of this sensor will be used.

Option to Compensate qc During Calculation of qr_hf and/or qr_rtc

While defining the terms for calculating qr_hf and qr_rtc, the user can decide if qc (the heat flow due to a calibration heater) should be compensated or not.

Quick Reporting and Data Exchange

Print Functionality Added to Many Screens

The option to send a screenshot directly to a printer has been added to many of the displays within iControl. This functionality can be used to print a screenshot on paper or to transfer a screenshot to an ELNB (electronic laboratory note book) provided this is installed on your system as a printer.

Printable Sensor History Report

Within iControl RC1e 5.0 it is now possible to print a detailed sensor history report, regardless of whether the sensor is connected to the RC1*e* itself or to a RD10, RTCal or UCB box. The report contains offset and slope data and the date and type of the last adjustment for each sensor.

New Functionality for the Chemical Database

The chemical database has been enhanced with some new functionality to improve its usability:

- Chemicals can now be assigned to groups – for example, chemicals can be structured into acids, bases, solvents, catalysts, etc.
- Using the new "Comments" field, specific data in relation to a chemical (or a specific batch of this chemical) like the purity or the source of supply, can be stored together with the physical or chemical properties.
- The import and export behavior for chemicals has been improved and is now easier and more intuitive.

Chemical Database Is Shared between All iControl Versions and iC Kinetics

There is no need to manage more than one version of the chemical database on one computer if working with different versions of iControl or in combination with iC Kinetics. All applications share the same chemical database and access the same physical and chemical data.

Compatibility

Support of Windows Vista 64-bit and Windows 7 Added

iControl now fully supports the 32-bit versions of Windows Vista and Windows 7 as well as Windows XP SP3. Additionally, iControl Office provides support for 64-bit systems.

Updated Equipment Database

The equipment database that the user specifies and selects his METTLER TOLEDO equipment from, like reactors, covers and stirrers, has been updated and now contains the latest equipment offered by METTLER TOLEDO.