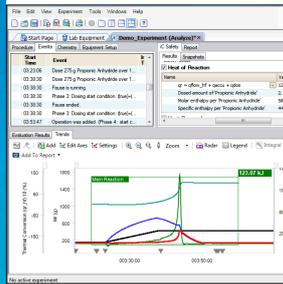


Evaluating Thermal Risk Streamline Safety Analysis



Safety results

Heat of Reaction

Name	Value	Unit
$q_{\text{rxn}} = \text{dflow}_{\text{JF}} + \text{accu}_{\text{J}} + \text{daccu}_{\text{J}}$	123.63	J
Dosed amount of Propionic Anhydride	2.115 mol	275.2 g
Molar enthalpy per Propionic Anhydride	58.16 kJ/mol	
Specific enthalpy per Propionic Anhydride	496.8 kJ/kg	

Heat Removal

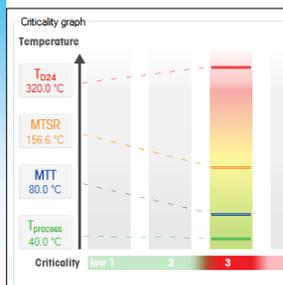
Name	Value	Unit
$q_{\text{removal}} = \text{dflow}_{\text{JF}} + \text{accu}_{\text{J}} + \text{daccu}_{\text{J}}$	113.713	J
Specific heat removal	267.9 kJ/kg	249 kJ/g
Specific heat removal rate	125.5 K	
Mean Value	125.5 K	
Max Value	125.5 K	
During reaction time (Integration range)	108.118	2707.167
During Dosing 1: 275.22 g at 17.95 g/min Propionic Anhydride	17.721 W/g	172.6 W/g

Adiabatic Temperature Rise (dTad) and MTSR

Name	Temperature	Time
ΔT_{ad} (Heat Removal)	125.5 K	
Maximum adiabatic temperature	268.5 °C	
MTSR (Heat Removal)	156.6 °C	03:37:26
None		

Thermal Accumulation

Name	Percent	Time
Thermal accumulation at stoichiometric pt.	89.89 %	03:37:26
Thermal accumulation at end of dosing	86.44 %	03:38:26



Process Understanding

A simple experiment using a Reaction Calorimeter provides reliable data to calculate safety relevant parameters, with the highest degree of confidence. iC Safety makes the conversion of experimental data into safety information simple, helping chemists and chemical engineers to understand the potential hazards of a chemical process faster.

Safety Analysis

The safety runaway graph describes both the desired and the undesired reaction in the event of a cooling failure. It factors in the most important safety information, is easy to interpret, and provides the base for a full safety assessment. The safety runaway graph represents a fast check of the nature of thermal risks linked to a given process.

Risk Assessment

In-depth understanding of the exothermicity of a chemical reaction is essential to make adjustments to the process. iC Safety presents the thermal risk, such as thermal accumulation, $\Delta T_{\text{adiabatic}}$ or MTSR in a concise and understandable format, enabling the appropriate conclusions to be made and the necessary measures to be taken.

Inherently Safer Processes

The criticality graph in iC Safety is a visual representation of the most crucial temperatures of a process. It classifies the process based on four characteristic temperatures. The resulting criticality class is one of the bases which help the engineer to estimate the hazardous potential and define adequate measures to make the process safe.



iC Safety™ – Critical Safety Information in One Click

The chemical and pharmaceutical industries often use complex products and processes in which large amounts of energy can be released. Process development is concerned with risks related to scale-up and manufacturing the product. Knowing and understanding the potential risks is critical, and a pre-requisite for the safe manufacturing of chemical and pharmaceutical products.

iC Safety is an intuitive application that utilizes experimental data from the Reaction Calorimeters EasyMax, OptiMax, and RC1 and other calorimetric techniques. It is designed to speed up and simplify the calculation of thermal safety values associated with chemical reactions. Better understanding of the thermal risks help the engineer to estimate the hazardous potential more easily, and to develop safe chemical processes faster.

Evaluating Thermal Risk Streamline Safety Analysis

iC Safety is a crucial tool for evaluating the thermal risk of a chemical reaction at industrial scale. Designed for use by both non-expert and expert users, it summarizes key safety information in an easy-to-understand graphical and tabular format, while providing access to detailed safety data needed by expert users.

Transforming Data into Information

iC Safety uses well established algorithms* and procedures to automatically convert reaction calorimetry data into safety information. The basic iC Safety information can be complemented with experimental data from other calorimetric measurements, such as DSC or adiabatic calorimetry as well as properties of the reaction mixture, to increase its significance.

Characterize the Risk

The severity of a runaway reaction is directly linked to the energy of the reaction. Hence, the adiabatic temperature rise in case of a cooling failure, the maximum temperature of the synthesis reaction (MTSR) or maximum achievable temperature (MAT) are important parameters to know. When the basic iC Safety information of the desired reaction is combined with data from the undesired reaction, the hazardous potential of the chemical can be described in a more detailed way, and the necessary conclusions can be drawn.

The information obtained is presented as numbers, trends and schematics that correlate to the relative position of critical temperatures. iC Safety automatically converts them into important charts known as "Safety Runaway Graph" and "Criticality Graph".

How it Works

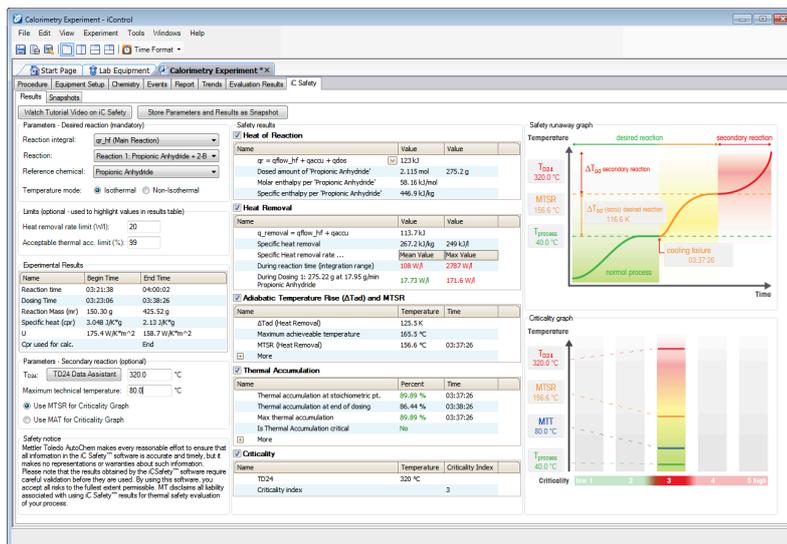
Following the basic evaluation of experimental data and reaction chemistry, iC Safety calculates the relevant safety parameters for the desired reaction. The results are presented conveniently in a table and the "Safety Runaway Graph" is created.

The T_{D24} assistant helps the user to integrate data from either DSC, ARC or other calorimetric techniques describing a potential secondary reaction that may occur in case of a cooling failure. In the event of multiple evaluations, all data sets are captured in a convenient table to allow simple comparison of the result sets.

Requirements to Operate iC Safety

- Reaction Calorimeters EasyMax, OptiMax, and RC1 with either the option "Heat Flow" or for RC1_e also with "RTCa"
- iControl 6.0 or newer (for EasyMax, OptiMax, RC1mx) or 5.3 and 5.6 (for RC1_e) software

* Thermal Safety of Chemical Processes, Francis Stoessel, Wiley-VCH, 2008, ISBN: 978-3-527-31712-7



Technical Specifications

PC Requirements	ONE iControl Application with ONE Instrument/Reactor	MULTIPLE iC/iControl Applications with MULTIPLE Instruments/Reactors
Operating System	32/64 bit versions of Microsoft® Windows® 7, 8.1, and 10	
CPU	Intel® Core™ i5 2.2 GHz or better	Intel® Core™ i7 Quad Core 2.2 GHz or better
Memory	8 GB or more RAM	16 GB or more RAM
Hard Drive	SATA 5400 rpm	Solid State Drive (SSD)
Graphics	SXGA 1280 x 1024 with 3D hardware acceleration	SXGA 1280 x 1024 with 3D hardware acceleration
Additional Software	Internet Explorer® 8.0 Web browser or newer, Microsoft® Office® 2007 or later, and the latest version of Adobe® Reader® or other PDF reader	

*Microsoft and Windows are either registered trademarks or trademarks of Microsoft Corporation in the United States and/or other countries.

Unsupported Experiments

iC Safety 6.0 is not applicable to experiments carried out with iControl 5.3 or 5.6 containing calorimetry information.



Accelerate Development with iC Suite

The iC Suite of software products support METTLER TOLEDO *in situ* spectroscopy, particle system characterization, precise reactor control 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

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