# Increase Safety Knowledge Calorimetry from Screening to Production







# **Understand Process Parameters**

EasyMax and OptiMax HFCal combine the benefits of a synthesis workstation and a reaction calorimeter. Thermodynamic information, such as heat transfer, specific heat, heat flow or enthalpy are collected under both isothermal and nonisothermal conditions, ensuring process parameters are understood.

## **Uncover Potential Safety Issues**

Critical information, like induction time, start and end of reaction and maximum heat release, combined with more detailed information, such as reaction enthalpy, accumulated energy and adiabatic temperature rise on cooling failure, ensures potential safety issues are quickly identified.

## Faster Process Development

Characterize and optimize process parameters in a controlled, accurate and reproducible environment. Collecting safety relevant heat information simultaneously reduces the number of trials – saving time and resources.



#### Data Analysis

During an experiment EasyMax and OptiMax HFCal collect and store a wealth of information. iControl software automatically calculates and reports heat transfer data, specific heat of the reaction mass, heat flow and reaction enthalpies.



### EasyMax<sup>™</sup> and OptiMax<sup>™</sup> HFCal

Uncovering potential safety issues or non-scalable conditions are essential to develop and scale a process safely. However, this information is not typically generated until late in the scale-up phase.

The smaller EasyMax HFCal provides reaction safety information early in development, while the larger OptiMax HFCal determines heat and scalability details to safely scale processes. Both calorimetry workstations provide heat release data, reaction enthalpy and heat transfer as well as specific heat data enabling chemistry and process decisions to be made earlier – resulting in faster process development and safer scale-up.



# **Technical Specifications**

Thermostat	EasyMax 102 LT HFCal	EasyMax 102 HFCal	EasyMax 402 HFCal	OptiMax HFCal
Heating/Cooling	Electrical/Peltier			
Temperature Range	–90 °C to 80 °C (jacket temperature)	-40 °C to 180 °C (jacket temperature)		
Control Modes	sothermal and isoperibolic, constant or ramp, reflux, distillation and crystallization			
Stirring	50 rpm to 1000 rpm			30 rpm to 1200 rpm
Dimensions (Thermostat) WxDxH	430 mm x 360 mm x 280 mm	330 mm x 360 mm x 280 mm	430 mm x 360 mm x 280 mm	388 mm x 414 mm x 539 mm
Power Supply	100 V to 240 V AC, 50 Hz to 60 Hz, 1000 VA			100 V to 240 V AC, 50 Hz to 60 Hz, 1300 VA
Operation	Touchscreen and iControl software for calorimetric applications			
Reactors				
Type/Material	Single-piece or two-piece (Borosilicate glass)			
Working Volume	40 mL to 100 mL	-	80 mL to 400 mL	150 mL to 1000 mL
Pressure	50 mbar to 1 bar			
Stirrer	Magnetic stir bar; Pitch-blade (glass, Alloy C-22); Anchor (glass, Alloy C-22); Half-moon blade (PTFE blade; glass, PTFE or Alloy C-22 stir shaft – for single-piece reactor) Pitch-blade (glass, Alloy C Half-moon blade (PTFE blade; glass, for single-piece reactor)			C-22); Anchor (glass, Alloy C-22); ade; glass, PTFE or Alloy C-22 stir shaft –
Calorimetry: Heat Flow				
Precision Heat Transfer <sup>1</sup>	Typically $\pm 4\%$			Typically ± 3%
Accuracy and Precision Specific Heat <sup>1</sup>	Typically ± 12%			Typically ± 10%
Accuracy Heat Flow <sup>1</sup>	Isothermal conditions: $\pm$ 3% to 5%; Non-isothermal conditions: $\pm$ 5% to 10%; Based on comparison of qr_hf with qc resp. $\int qr_h f$ with $\int qc$ .			Isothermal conditions: ± 3% to 5%; Non-isothermal conditions: ± 5% to 10%; Based on comparison of qr_hf with qc resp. ∫qr_hf with ∫ qc.
Sensitivity qr Noise <sup>1</sup>	≤ 0.2 W equivalent to 2 W/L		≤ 0.25 W equivalent to 0.6 W/L	≤ 0.4 W equivalent to 0.4 W/L
HFCal Module	• •			
Power and Data Interface	Direct connection to CAN interface of standard EasyMax/OptiMax, no additional power supply or PC connection required			
Data Logging	Via iControl software			
Dimensions, WxDxH	120 mm x 40 mm x 170 mm			
Software				
iControl	iControl 6.1 or higher, HFCal license required	iControl 5.2 or higher, HFCa		
Calibration Heater				
Power Rating	Max. 10 W			Max. 20 W
Material	Alloy C-22			· ·
Size	Ø 6 mm, 260 mm length			Ø 8 mm, 300 mm length

<sup>1</sup> Data determined with ethanol between -65 °C and 25 °C, toulene between -35 °C and 75 °C, silicone oil 47 V 20 between -25 °C and 160 °C, water between 5 °C and 40 °C

# **Product Configurations**

To perform calorimetric studies, the Upgrade Kit, the Software Option as well as the iControl software are required.

#### 30090576

#### Upgrade Kit EasyMax HFCal

A calorimetry Upgrade Kit for EasyMax contains all necessary parts to convert the workstation into a fully functional calorimeter (needs software).

#### 30720937

#### Software EasyMax HFCal Option iControl

Software option enabling calorimetric experiments and heat flow evaluations in iControl.

#### **METTLER TOLEDO Group**

Automated Reactors and In-situ Analysis Local contact: www.mt.com/contacts

#### 30050150

#### Upgrade Kit OptiMax HFCal

A calorimetry Upgrade Kit for OptiMax. It is plug-and-play and contains all necessary parts to convert the workstation into a fully functional calorimeter (needs software).

# 30720936

# Software OptiMax HFCal Option iControl

Software option enabling calorimetric experiments and heat flow evaluations in iControl.

www.mt.com/HFCal

For more information

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