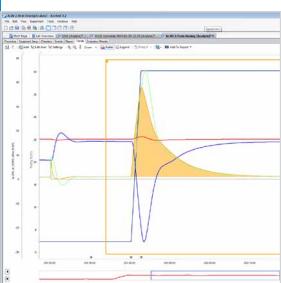


# Understand Process Parameters

## Faster, Safer Process Development



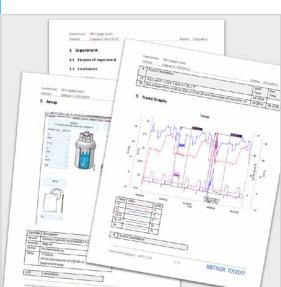
**Understand Process Parameters**  
OptiMax HFCal combines the benefits of a synthesis workstation and a reaction calorimeter, collecting heat data for scale-up and safety information. Heat data under both isothermal and non-isothermal conditions enables measurement and optimization of process parameters under process-like conditions.



**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 well-controlled, accurate and reproducible environment. Collecting safety relevant heat information at the same time reduces the number of trials – saving time and resources.



**Data Analysis**  
During an experiment OptiMax HFCal collects and stores a wealth of information. With a single click, iControl software automatically calculates and reports heat transfer data, specific heat of the reaction mass, heat flow and reaction enthalpies.



### OptiMax™ HFCal

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

OptiMax HFCal is a synthesis workstation designed specifically to enable the determination of this critical information much earlier in the development process. Reaction enthalpy, heat transfer and maximum heat release data is collected and calculated in a simple way, enabling better decisions to be made earlier regarding chemistry and conditions – ultimately resulting in faster process development and scale-up.

## Understand Process Parameters

### Faster, Safer Process Development

#### Heat Flow Calorimetry – Simple and Accurate

OptiMax HFCal reproducibly delivers information to characterize process parameters, for scale-up and to ensure it is safe at scale.

- Heat transfer coefficient
- Specific heat of the reaction mass
- Heat flow for isothermal and non-isothermal conditions
- Enthalpy
- Thermal conversion
- Adiabatic temperature rise

#### Heating and Cooling – No Additional Cryostat Needed

The electrical heating and Peltier cooling ensure precise temperature control from  $-40^{\circ}\text{C}$  to  $180^{\circ}\text{C}$ . It doesn't require any cumbersome or bulky cryostats.

#### Quality Information

All events and data are recorded automatically, making experiments traceable and reproducible. At the end of the experiment, the relevant data is summarized and a report with tables and trends is generated automatically. For further processing, interpretation or storage purposes, the data are either taken care of by iC Data Center™ or can be exported to Microsoft® Excel®.

#### 30064130 – OptiMax Calorimetry Starter Kit

The OptiMax HFCal Starter Kit is a heat flow based, ready-to-use system to quickly obtain heat data of any chemical or physical reaction on a 1 L scale. This includes all parts required plus iControl software and HFCal license.

#### 30050150 – OptiMax HFCal Kit

The OptiMax HFCal Kit is a calorimetry upgrade kit for OptiMax. It is Plug&Play and contains all necessary parts to convert the workstation into a fully functional calorimeter. iControl software is not included. No service call is required for installation.

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#### OptiMax HFCal Specifications

##### Thermostat

|                     |   |      |
|---------------------|---|------|
| Heating             | Electrical  |      |
| Cooling             | Peltier   |      |
| Cooling Performance | 0 °C  | 35 W |
|                     | 20 °C   | 65 W |
|                     | 40 °C   | 90 W |
| Temperature Range   | $-40^{\circ}\text{C}$ to $180^{\circ}\text{C}$ (jacket temperature)                               |      |
| Control Modes       | Isothermal and isoperibolic, constant or ramp, reflux, distillation and crystallization           |      |
| Stirring            | 30 rpm to 1200 rpm  |      |
| Dimensions          | 388 mm x 414 mm x 539 mm  |      |
| Power Supply        | 100 V to 240 V AC, 50 Hz to 60 Hz, 1300 VA  |      |
| Operation           | iControl software for calorimetric applications<br>Graphical touchscreen and/or iControl software |      |

##### Reactors

|          |  |
|----------|--|
| Type     | Single piece or two piece (with bottom drain valve)  |
| Volume   | 1000 mL  |
| Pressure | 50 mbar to 1 bar   |
| Material | Duran® glass   |
| Stirrer  | Pitch-blade (glass, Alloy 22), Anchor (glass, Alloy 22), Half-moon (PTFE for single piece reactor) |

##### Calorimetry

|                           |   |
|---------------------------|---|
| Type                      | Heat flow   |
| Precision Heat Transfer** | Typically $\pm 3\%$   |
| Accuracy and Precision    | Typically $\pm 10\%$  |
| Specific Heat**           |   |
| Accuracy Heat Flow**      | Typically $\pm 3\%$ to $5\%$ , under isothermal conditions.<br>Typically $\pm 5\%$ to $10\%$ under non-isothermal conditions.<br>Based on comparison of $qr_{hf}$ with $qc$ resp. $\int qr_{hf}$ with $\int qc$ . |
| Sensitivity qr Noise**    | $\leq 0.1\text{ W}$ measured as standard deviation of $qr$ under steady state conditions.<br>Peak-to-peak noise is $\leq$ approximately $0.4\text{ W}$ .  |

##### HFCal Module

|                          |  |
|--------------------------|--|
| Power and Data Interface | Direct connection to CAN interface of standard OptiMax, no additional power supply or PC connection required |
| Data Logging             | Via iControl software  |
| Dimensions               | 120 mm x 40 mm x 170 mm  |
| Software                 | iControl 5.2 or higher, HFCal license required   |

##### Calibration Heater

|          |                              |
|----------|------------------------------|
| Power    | Max. 20 W                    |
| Material | Alloy 22                     |
| Size     | 300 mm length, 8 mm diameter |

\*\* Data determined with silicon oil 47V20 between  $-25^{\circ}\text{C}$  and  $160^{\circ}\text{C}$ , water between  $5^{\circ}\text{C}$  and  $40^{\circ}\text{C}$ , toluene between  $-35^{\circ}\text{C}$  and  $75^{\circ}\text{C}$ .

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For more information