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Reaction Calorimetry

For Process Development and Safety

HEL
better chemistry – faster

Want to increase
use by R&D
chemists?

Want to improve
methodology for
specialists?



Calorimetry theory has been imbedded into HEL's proprietary reactor control software to allow direct and on-line display of heat release as reaction proceeds.

In order to increase use by R&D chemists, simplifications based on sound data and over 20 years experience have been incorporated while for those looking for accurate data, full and complete theory has been retained but with time-saving calculations still done on-line and in real-time.

... Flexible, Adaptable, Modular ...

Reaction Calorimetry enables ...

Reaction tracking

- ▲ Determine end-of-reaction on-line
- ▲ Track on-line, changes in reaction rate or mechanism
- ▲ Directly compare different routes or process changes
- ▲ Determine if reaction is feed or kinetic controlled

Process Safety

- ▲ Cooling duty needed
- ▲ Potential temperature/pressure rise

*Calorimetry is now accessible
to development chemists on
ANY stirred reactor without
special features or
adaptations.*

...Online, Real-time, Affordable...

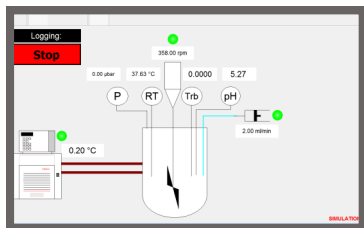
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Calorimetry for R&D chemists

Considerable development effort has been expended in developing methodology that will encourage large numbers of chemists to embrace calorimetry as additional insight into their process without ANY extra hardware or additional experimental time being necessary. The key features are the following:

Basis

- ▲ No knowledge of methodology or theory required
- ▲ May be used with minimal or even zero user input
- ▲ Data displayed in real-time as reaction is performed
- ▲ No extra experimental time required
- ▲ No off-line analysis/calculations needed



Turn simple existing reactors into automated systems at minimum cost—compact control unit with touch screen interface

Hardware

- ▲ Existing or new, jacketed reactors
- ▲ Special software interface for chemists averse to computer control
- ▲ Software implementation on a PC or special microNOTE touch-screen monitor
- ▲ Compact design to suit already crowded fume hoods

Special Features

- ▲ “HF” meter supplied to allow confirmation of data
- ▲ On-site training by experienced chemists
- ▲ Software for complete automation of reactor
- ▲ Ability to expand system



Calorimetry for “serious” or specialist applications

HEL’s propriety SIMULAR reaction calorimeter is now supplied with this new on-line methodology in place, allowing high level calorimetry analysis but without the need for time consuming experimentation or specialist off-line analysis. Key features are:

- ▲ Sound calorimetry theory and well researched methodology to provide accurate results
- ▲ Custom electronics and reactor hardware
- ▲ On-line calculation of heat release, in real time
- ▲ Choice of heat flow and power compensation calorimetry

Key benefits compared with conventional reactor calorimeters include:

- ▲ No time lost for UA calibrations (with power compensation)
- ▲ No off-line calculations (even for heat flow)
- ▲ All calculations are automated and on-line, real-time
- ▲ Fast control and accurate results

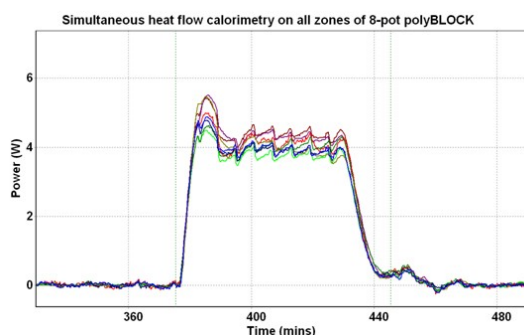


On-line/ Off-line Calorimetry Comparison (Acetic anhydride dosed into water at 40°C)

	Reaction Energy (kJ)	Dose Energy (kJ)	Molar Heat (kJ/mol)
On-line before final baseline correction	62.2	5.5	52.9
On-line after final baseline correction	71.3	5.5	59.9
Off-line calculation	71.3	5.5	59.9

Calorimetry for parallel applications

HEL’s simplified heat flow methodology can also be implemented on multiple reactor systems, giving on-line and real time results in parallel. This has already been implemented on HEL’s PolyBLOCK and AutoMATE platforms and typical results are shown.



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