

Application Note

The use of FlexyPAT-HFC for calorimetric measurements

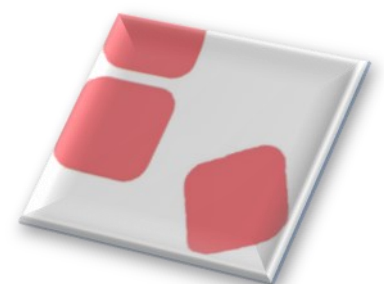
Regardless if you need to do process safety measurements for scale-up studies, kinetic analysis for process optimization, etc., with FlexyPAT-HFC you have a strong and flexible tool in your laboratory.

FlexyPAT is a modular Process Automation Technology that enables automated customer-specific lab reactor systems to be implemented in a very cost-effective manner, including with the integration of existing devices.

The option „Heat-Flow-Calorimetry“ converts, within a few minutes, a standard SYSTAG FlexyPAT system into a sophisticated Heat-Flow calorimeter . The design and performance of this easy-to-use calorimeter fulfills the basic requirements in typical R&D laboratories.

Performance

- ⇒ Isothermal Heat-Flow Calorimeter with optionally Heat-Balance for reflux-condenser.
- ⇒ Flexible system for different reactors from 500ml up to 5l, glass or steel vessels.
- ⇒ Intuitive Recipe Control Software allows changes “on-the-fly”.
- ⇒ Integration of third-party technology like turbidity, FT-IR, particle-size analyzer, sampling Systems, ultrasonicators, etc.





Functionality

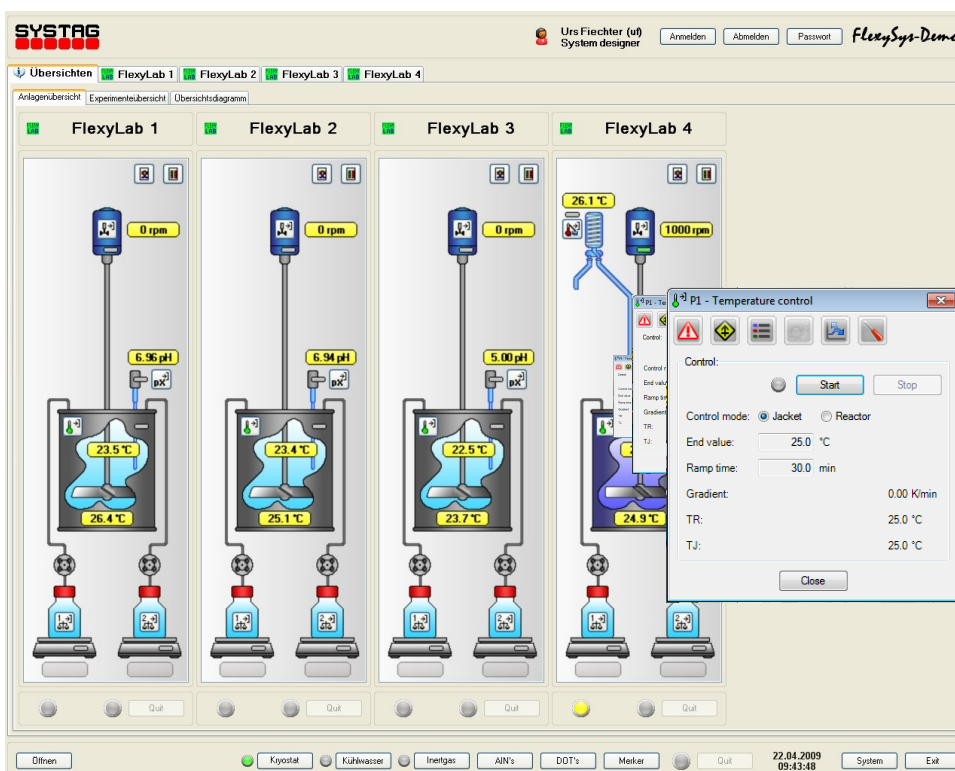
FlexyPAT is a flexible system, that allows customised functionality. The basic system includes:

- ⇒ Temperature control, jacket or reactor mode
- ⇒ Stirrer speed control and torque measurement
- ⇒ 2 dispensing (gravimetric or volumetric)
- ⇒ pH-control (pX-control)
- ⇒ Automatic distillation^[1] / pressure-vacuum control^[1] / hydrogenation^[1] / automatic solubility^[1]



The base of success

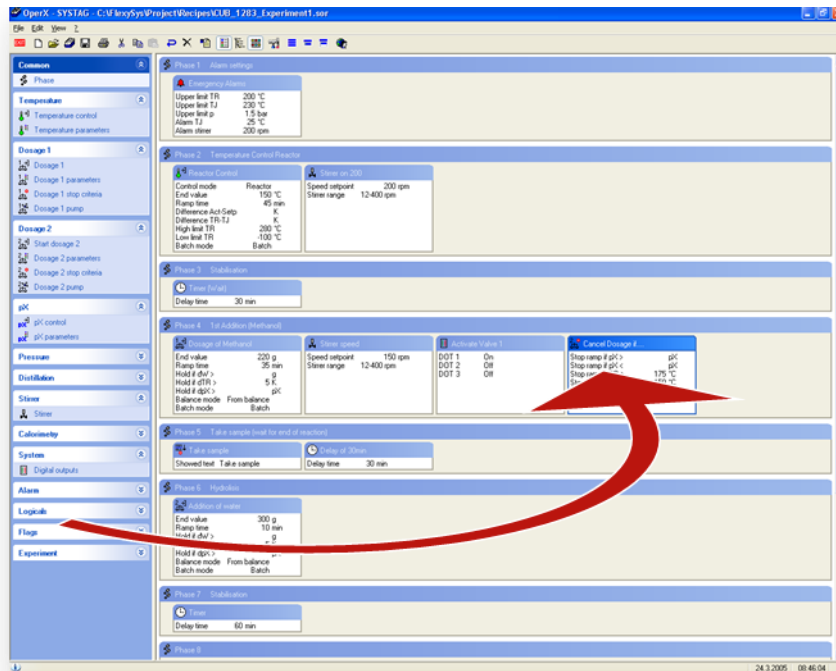
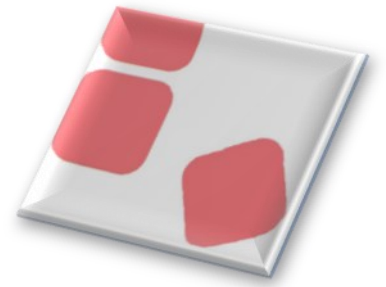
Apart from the standardised lab-glassware, the intuitive and user-friendly software is another productive features of FlexyPAT. Not only specialists but also newcomers in calorimetry will become familiar with this system within a short period of time! A key-figure of the world-wide success of all the SYSTAG applications is the very intuitive software.



This picture shows the graphic interface of simultaneous reactor operations. Up to 6 reactors in parallel, each with 2 gravimetric feed can be controlled on 1 PC. (Here, 4 are shown.)

By manual operation every function (T-control, dosage, stirrer) is activated by a simple click on its symbol to open a sub-window with further parameters. Data logging & trending is possible at any time during the process.

^[1]optional



The included Batch-Recipe-Editor is based on “Drag & Drop” MS-Windows technology.

All existing operations (Temp, Dosage, Stirrer etc.) are listed in the table on the left side. A new recipe is created by drag & drop functionality.

Often used sequence of steps and operations may be stored as a “method” and can be added at any place in a recipe.

No better way to create SOP (Standard Operation Procedures)! Changes “on-the-fly” are possible, as well as manual interaction by the user. The report file recognizes all the events.

Calorimetric results

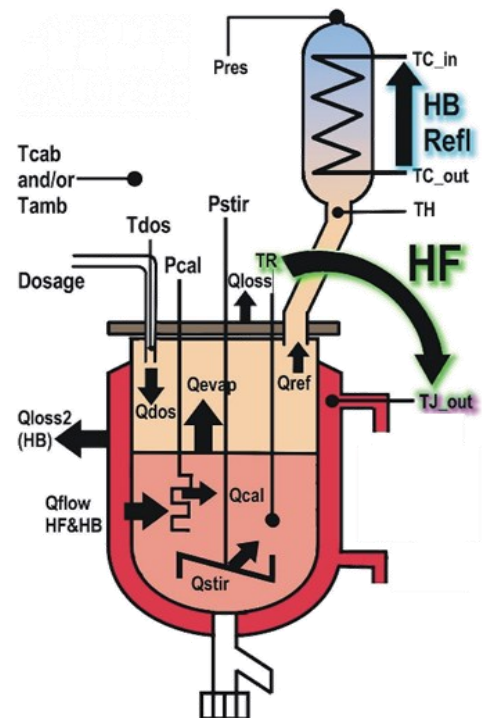
All SYSTAG calorimeters provide the following results:

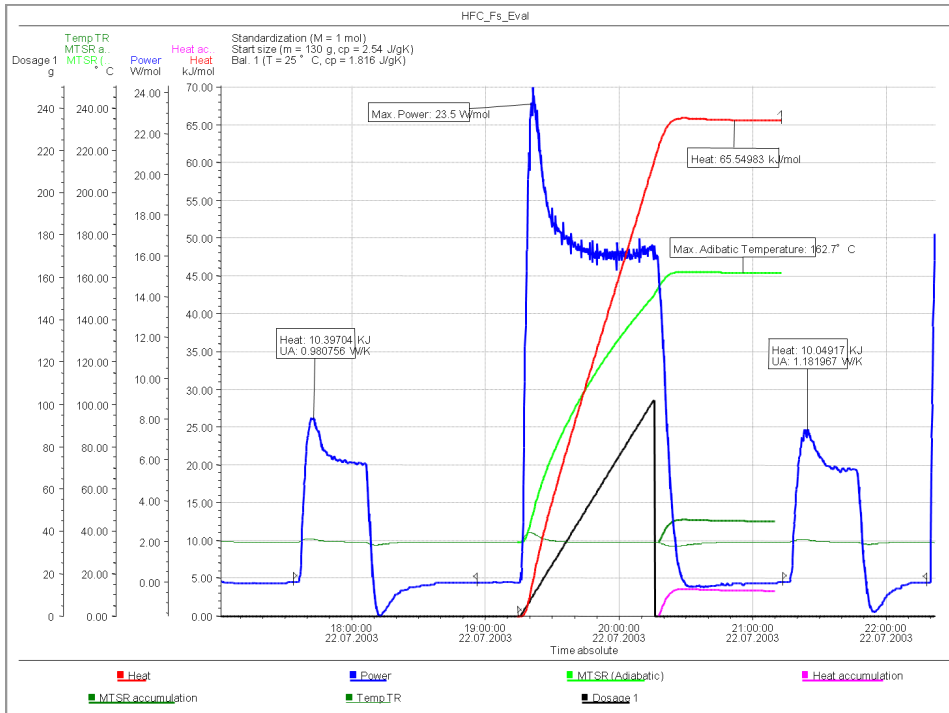
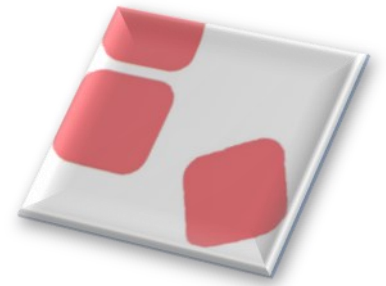
- ⇒ Heat & power of reaction
- ⇒ Adiabatic temperature rise (MTSR)
- ⇒ Accumulation of reaction

In combination with the option “Heat Balance Calorimetry,” the above mentioned results are given separately for the reflux condenser term for reaction at the boiling point.

All these results are not only given as numeric values but also displayed in a chart (see next page).

The isothermal heat-flow calorimetry is the most common technology for reaction calorimetry in Safety and R&D Laboratories.





The diagram to the left shows all the necessary results for process safety analysis and/or for kinetic studies.

Blue = Power of reaction
 Red = Heat of reaction
 Green (bright) = (MTSR) Adiabatic temp. increase
 Black = feed
 Green (dark) = Process Temp
 Heat accumulation

Power & Heat of Reaction: From the graph it is possible to read the maximum Power and Heat given by the reaction.

Adiabatic Temperature: The MTSR (maximum temperature by synthesis reaction) displays the worst-case for the present experiment. Assuming a cooling failure, the process temperature (35°C) could increase under adiabatic conditions up to about 160°C (green bright).

Accumulation: It is important to understand the accumulation of a Process. By the above shown graph, it is easy to distinguish between total heat (red) and accumulation (pink). The present experiment accumulates by about max. 10% (compare pink and red curve).

Run-away Reaction & Critical Class: Further analysis like Run-away Scenario or classification regarding the Critical Classes of reaction can be done, based on the above shown results.

SYSTAG supports you to evaluate the most relevant equipment for all your needs in the scope of Controlled Lab Reactors, Thermal Process Safety and Plant Control Systems.

