Reproducible experiments for reaction optimization

New generation of parallel synthesis reactor

Temperature control at high speed to the point: 10 reaction preparations in a single unit. Precise and completely independent heating, cooling and stirring

In order to obtain meaningful results in solubility determination, catalysis reactions, crystallization experiments and PCR reactions, the experimental conditions, the experimental procedure and a protocol are essential.

Requirements on the reproducibility of experiments can often not be sufficiently fulfilled.

Meaningful experiments for parallel synthesis, process optimization and DoE studies require conditions that are as reproducible as possible with regard to the relevant reaction parameters. In addition to concentrations, pressure and other environmental conditions, temperature, temperature profiles and uniform mixing are the essential factors to ensure constant or comparable reaction conditions.

Conventional synthesis instruments can usually only set fixed parameters (e.g. stirring speed or temperature) for all reaction cells due to their design. In some systems, the reproducibility in the temperature profile, both over time and between reaction cells, may not be sufficiently high, since the cooling and heating capacities may vary.

Users* who need very flexible, variable and above all very easy to operate instruments for carrying out organic synthesis reactions have not had an easy time so far. In order to be able to reproduce the diverse reaction conditions, up to now it has been necessary to make concessions in terms of flexibility or operability.
For reaction preparations between 2 ml and 30 ml, there are few solutions on the market for controlled and monitored systems. The demand for reaction volumes well below 100 ml is increasing. It is advantageous to offer the same monitoring and control possibilities as are usual for larger systems in the scaling-up and kilo laboratory.

The XELSIUS synthesis reactor was developed to provide optimal and practical solutions for many tasks.

Space-saving process optimization - 10 reactors in just one unit.

With a weight of 12.7 kg and a length of 36 cm at a height of only 14 cm, the XELSIUS synthesis reactor requires very little space in the fume cupboard. Furthermore, the monitor and control PC can be conveniently positioned outside the fume cupboard.

Durability and quality - 24/36 months warranty on the cells

When selecting the components for the reactor cells, e.g. Peltier elements, components are chosen that are optimized for durability and reliability.
In order to maximize the service life, the XELSIUS synthesis reactor has optimized control and power electronics for the cells. The thermal and electromagnetic loads on the Peltier elements are minimized. As standard, nevoLAB offers a 24-month warranty on the cells. For an additional charge, this warranty can be extended to 36 months.

Very high reproducibility and accuracy between cells.

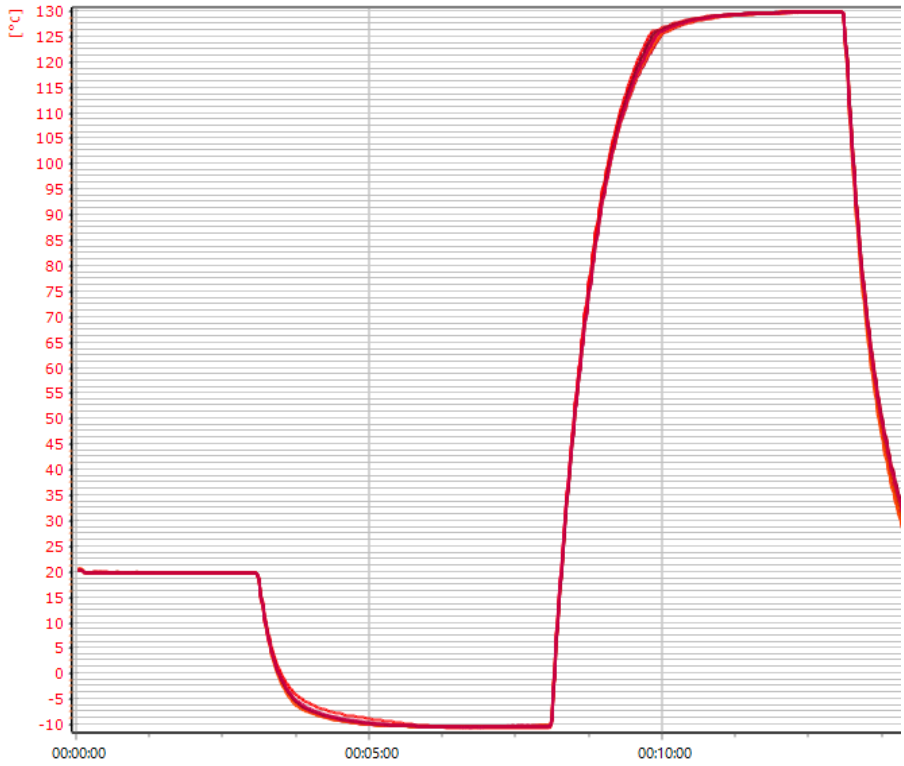


Figure: 1: Reproducibility at 10 parallel temperature profiles

The smallest deviations between the temperature profiles of the individual cells ensure a high degree of comparability in temperature-sensitive experiments. This is particularly useful for:

- Solubility determinations
- Catalysis reactions
- Crystallization experiments and in
- PCR reactions.

The range of jacket temperatures between the individual cells in the XELSIUS synthesis reactor varies within a range of +/- 0.25 K.

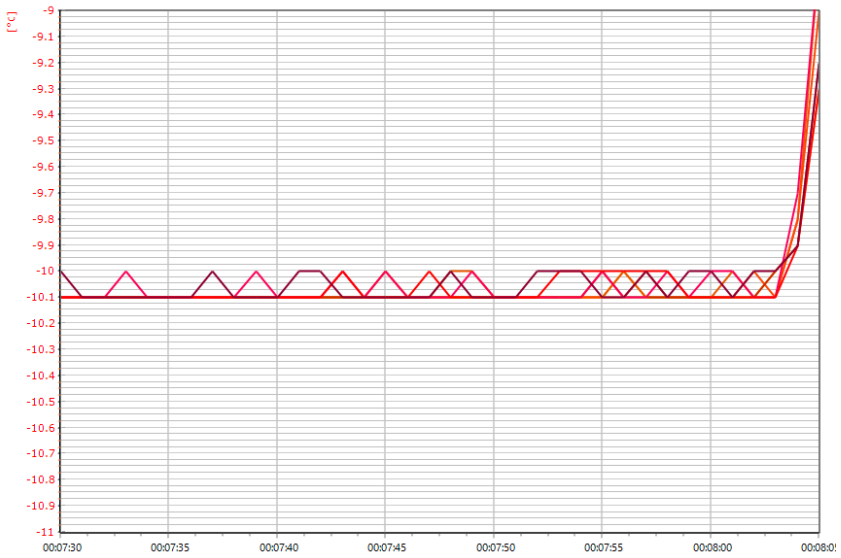


Figure 2: Spread of about 0.1 K for ten reactor cells operated in parallel at the target temperature of minus 10.0°C.

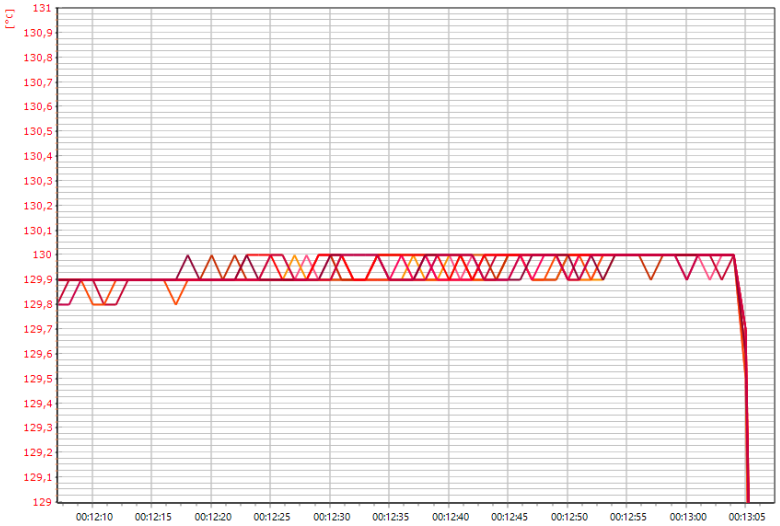


Figure 3: Variation of about 0.2 K for ten reactor cells operated in parallel at the target temperature of 130.0°C.

Optimized for fast and reproducible heating and cooling

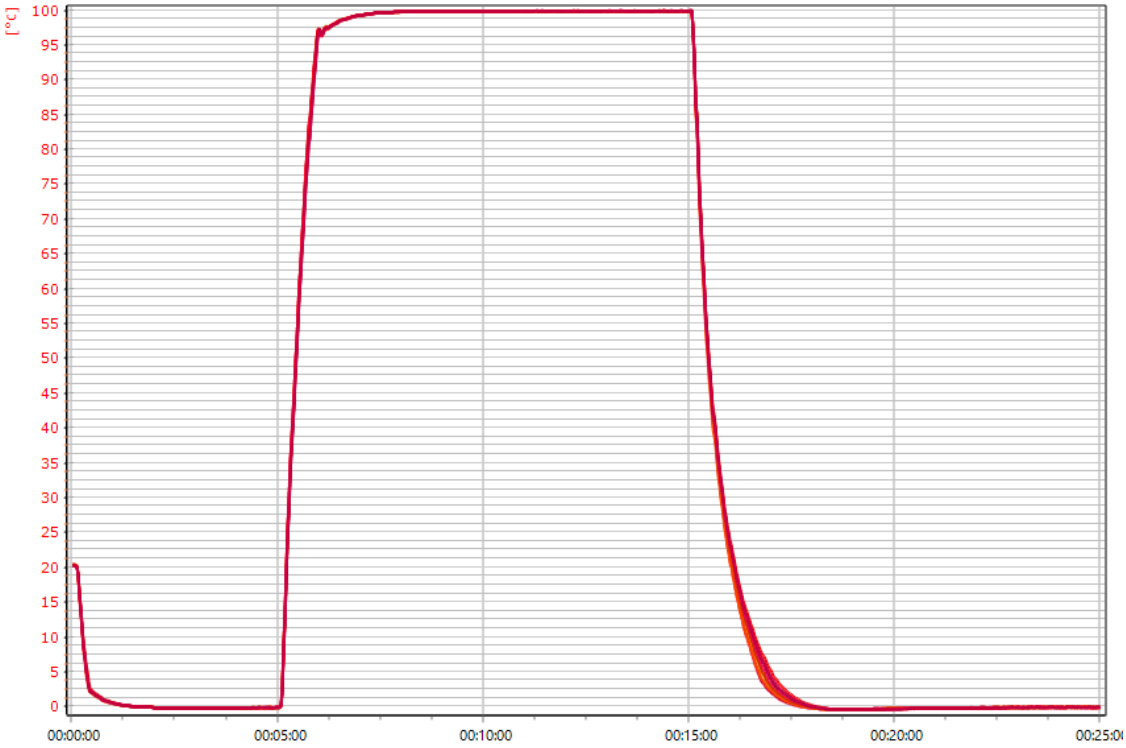


Figure 4: Reproducibility during rapid heating and cooling with ten reactor cells running in parallel.

The XELSIUS synthesis reactor was designed to allow the fastest possible temperature changes. The latest materials are used in the construction. In combination with high-performance Peltier elements, the XELSIUS synthesis reactor enables very fast and reproducible heating rates of the jacket temperature. Heating from 0°C to 100°C takes less than two minutes, which corresponds to a heating rate of more than 50 K/min.

In the case of cooling from 100°C to 0°C only about three minutes are needed.

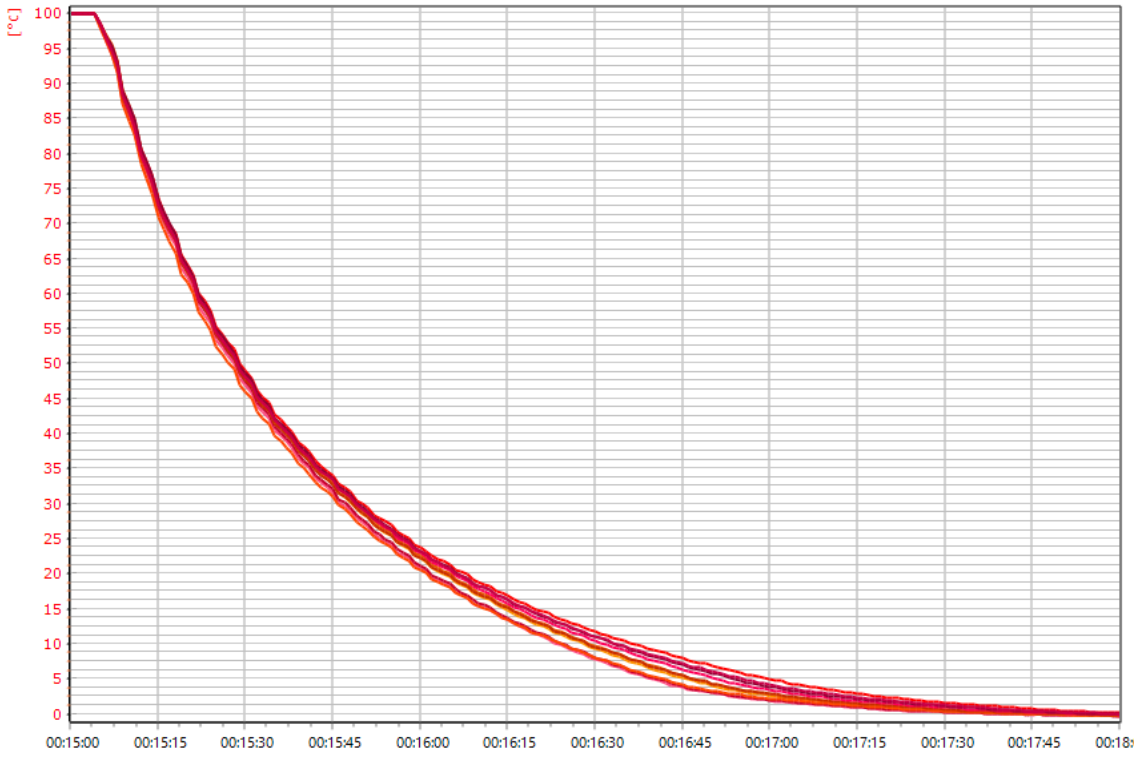
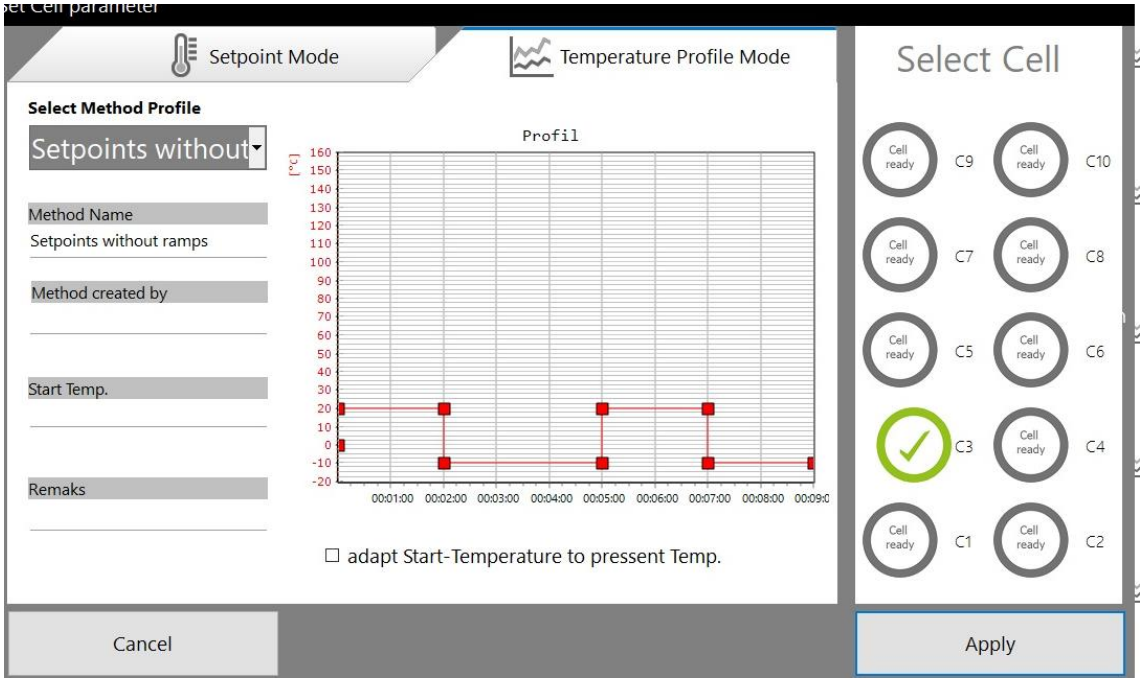


Figure 5: Fast and reproducible cooling at about 30 K/min from 100°C to 0°C with ten reactor cells operated in parallel.

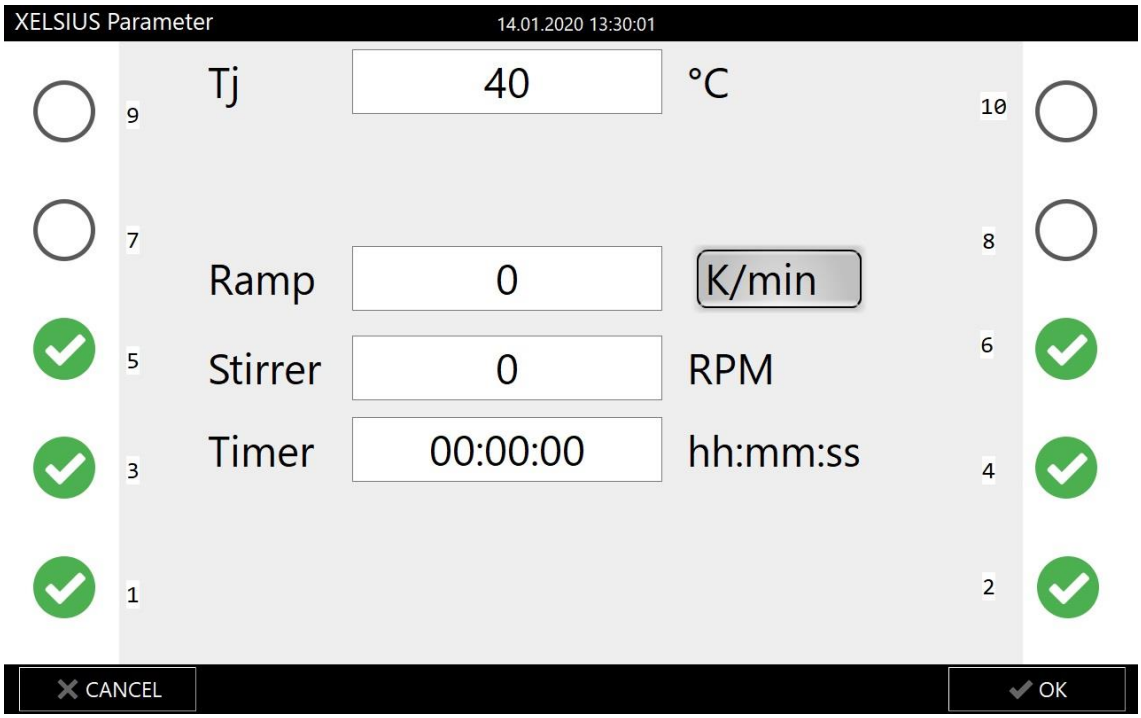
Heating programs with up to 100 steps and ramps can be defined in the software. The possible heating/cooling rates range from 1 K/h up to the technically maximum achievable values.

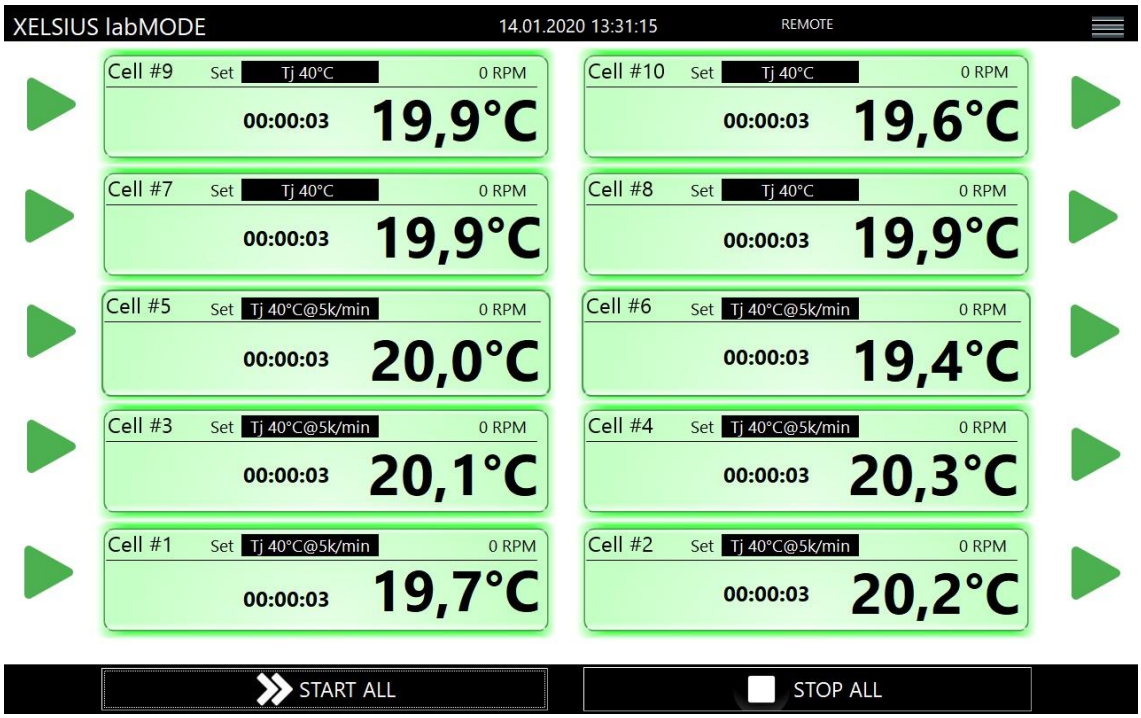


With the LAB MODE, the XELSIUS Synthesis Reactor can be operated as easily as a hotplate with magnetic stirrer.

The XELSIUS synthesis reactor reports directly in the so-called "LABmode" screen after switching on.

Each individual reactor cell can be selected very easily and intuitively. The temperature, time, stirring speed and a ramp can be set very easily.


XELSIUS Parameter
14.01.2020 13:30:01
Tj
40
°C
9
10
7
8
Ramp
0
K/min
5
Stirrer
0
RPM
6
3
Timer
00:00:00
hh:mm:ss
4
1
2
CANCEL
OK


XELSIUS labMODE
14.01.2020 13:31:15
REMOTE
Cell #9 Set Tj 40°C 0 RPM
00:00:03
19,9°C
Cell #10 Set Tj 40°C 0 RPM
00:00:03
19,6°C
Cell #7 Set Tj 40°C 0 RPM
00:00:03
19,9°C
Cell #8 Set Tj 40°C 0 RPM
00:00:03
19,9°C
Cell #5 Set Tj 40°C@5k/min 0 RPM
00:00:03
20,0°C
Cell #6 Set Tj 40°C@5k/min 0 RPM
00:00:03
19,4°C
Cell #3 Set Tj 40°C@5k/min 0 RPM
00:00:03
20,1°C
Cell #4 Set Tj 40°C@5k/min 0 RPM
00:00:03
20,3°C
Cell #1 Set Tj 40°C@5k/min 0 RPM
00:00:03
19,7°C
Cell #2 Set Tj 40°C@5k/min 0 RPM
00:00:03
20,2°C
START ALL
STOP ALL

Accessories and complete systems for special applications

By integrating external probes such as temperature probes or turbidity measurement sensors, the XELSIUS synthesis reactor can be expanded into a powerful complete system for special applications.

In combination with an automated sampling robot, special software has been developed for carrying out solubility determinations and crystallization experiments. This software allows not only the monitoring of turbidity but also the connection to an HPLC system for concentration determination.