h.e.l

Simular Reaction Calorimeter

For Process Safety and Development

Solutions in Process Safety

In industries ranging from pharmaceuticals to fine chemicals, there is a need to take small, laboratory scale chemical reactions to mass manufacture of a product.
It is necessary to identify and mitigate sources of risk during the process scale-up.
H.E.L provides a suite of safety scale-up tools to help you do this.

TSu

Phi-TEC I

Phi-TEC II

Simular

Your Problem

Our Solution

Discovery

Are these materials safe to proceed with?

Raw Material Hazard Screening
TSu
Phi-TEC I

Process Development

What operating conditions are required to minimize risk?

Reaction Calorimetry
Simular

Reaction Mix Hazard Screening
TSu

Scale-Up

What is the extent of the thermal risk?

What safety factors are required to mitigate worst-case scenarios?

Adiabatic and Reaction Calorimetry
Phi-TEC I, Simular

Hazard and Operability Assessment
Phi-TEC II

Manufacture

Isothermal Reaction Calorimeter

Simular

Central to the risks involved with scale-up are the changes in heat loss behaviour with scale:

- Many reactions are exothermic and require cooling to ensure safe operation when performed on a large scale;
- Components in the reaction may become unstable under certain operating conditions, leading to additional thermal hazards.

H.E.L's Simular is a highly configurable system that excels in optimizing process conditions and determining safer reaction conditions. With dual reactor options available, offering more flexibility for applications.

In addition to traditional heat flow calorimetry, the Simular offers power compensation calorimetry allowing direct measurement of the heat flow enabling operators to skip time-consuming calibration steps and get more conditions screened. The Simular is ideally suited for process safety and scale-up of the most varied and demanding reactions.

Measurement parameters for process safety, scale up and optimization

Process safety

- Reaction power (W)
- Reaction enthalpy (ΔH_r)
- Reaction kinetics
- Maximum temperature of synthesis reaction (MTSR)
- Mal-operations studies

Scale up data

- Heat accumulation
- Heat transfer rate
- Cooling duty
- Heat capcity data (MCp)

Process optimization

- Batch time and yield
- Batch cycle times

Direct drive agitation

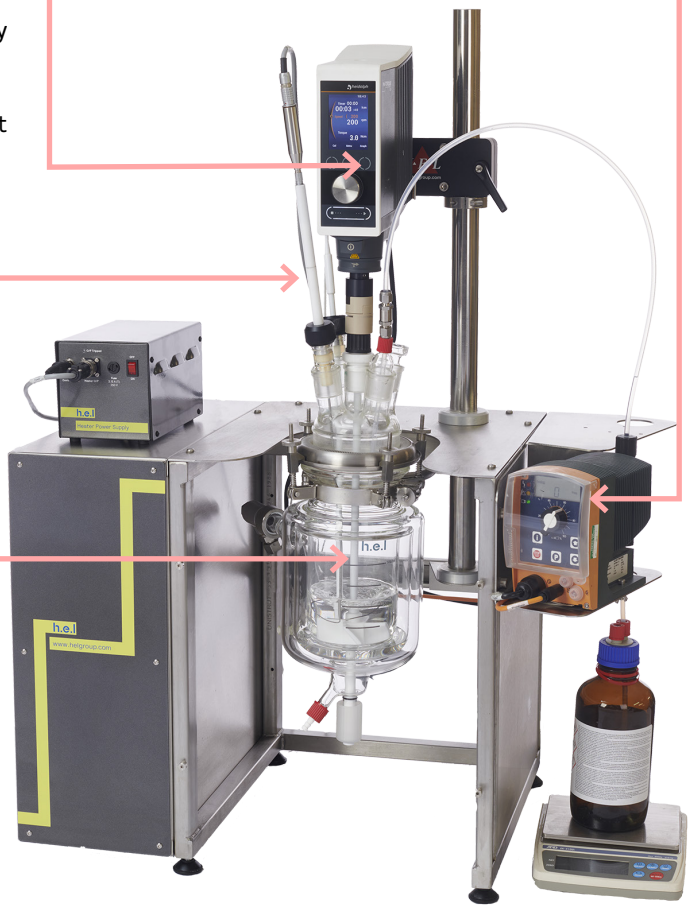
- Combined power, fine control and reproducibility for accurate and consistent results
- Impellers suitable for most reactions

Sensors / probes

- Accurate logging of temperature, pH and turbidity*
- Versatile hardware and software allows integration fo third-party sensors e.g. FTIR*

Reactors

- Available in a wide range of volumes and materials, with optimal volumes from 0.5 to 2L
- High pressure options available
- Designed for easy mounting and maintenance ensuring long-term

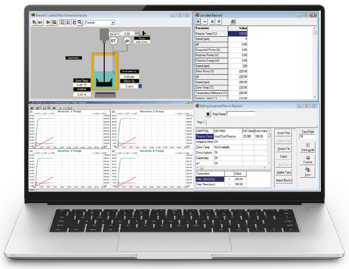


Feeds

- Fully configurable liquid and gas dosing protocols
- Customizable control loops – pH-hold
- Versatile sampling options

Software control

- Live display of all parameters
- Template-based user interface designed for both new and experienced users
- Robust safety features



*optional, contact your local sales rep for more information

Simular Applications

Process Optimisation

Yield, batch time

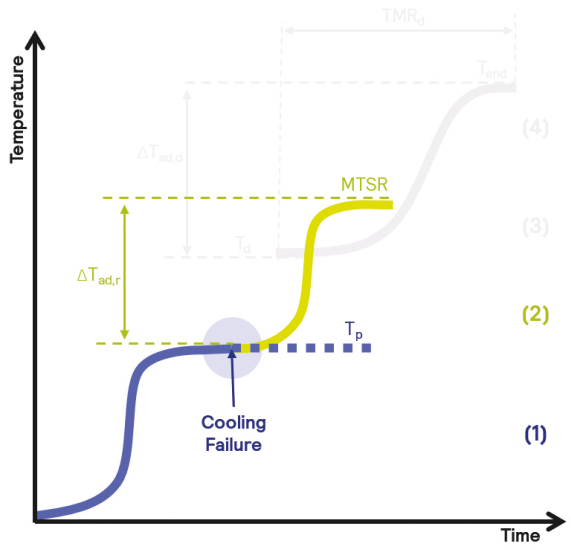
Achieve maximum yield and minimize side product formation with the advanced capabilities of Simular. The highly configurability and modularity of Simular system allows seamlessly integration with various sensors such as FTIR, turbidity, and particle sizing devices. By leveraging data from these diverse inputs, Simular provides a comprehensive understanding of your chemical processes, ensuring optimal performance and efficiency.

Minimizing Risk

Safer reaction conditions

Hazard assessments may identify insufficient process controls during normal operations and potential emergency situations caused by thermal runaway, aiming to mitigate the risk of such incidents. H.E.L's Simular can be used to explore and design safer reaction conditions, thereby also facilitating the optimization of safe operations and minimizing process risk.

Phases of Thermal Runaway



Thermal properties of the desired reaction (1)

The Simular measures the energy evolved in the reaction. Subsequently, this enables you to calculate the plant cooling capacity required to keep the reaction isothermal (T_p).

Thermal runaway of the reaction (2)

In the event of plant failure, it is critical to understand the maximum temperature the main reaction will reach during any subsequent thermal runaway.
The Simular enables the Maximum Temperature of Synthesis Reaction (MTSR) to be calculated from the data of the reaction. Multiple reaction conditions can also be screened to help understand the kinetics of the reaction. From this, it can be assessed whether there will be sufficient time and emergency cooling capacity to deal with the temperature increase.

Scale-up Data
Heat transfer, cooling duty

Information necessary for the scale-up of reactions is readily obtained from the Simular.
This includes the cooling duty (Q) for either jacketed reactors or reflux condensers and heat transfer rate (UA). For multi-phase reactions where mixing is crucial, aspects of agitation can also be studied.

Reaction Kinetics
Dose or kinetic controlled reaction

Simular provides heat release rate data which offers direct kinetic information, enabling quick assessment of whether a process is controlled by the rate of reagent addition or if the kinetics are the limiting factor. This valuable data helps streamline your analysis and improve process control.

Faster and more efficient Calorimetry

The Simular Reaction Calorimeter supports classic heat flow calorimetry, advanced calibration-free power compensation calorimetry, and reflux calorimetry. These advanced features allow users to choose the most appropriate method for their specific reaction requirements, ensuring accurate and reliable measurements for precise process control and optimization.

Heat Flow Calorimetry

The standard method for reaction calorimetry measuring the heat released or absorbed by a sample during a physical or chemical process. By monitoring the heat exchange with its surroundings, it provides insights into the sample's thermodynamic properties and reaction kinetics.

Power Compensation Calorimetry

This calorimetry method is ideal for when information on rapidly changing power output is required. The Simular's calibration-free approach enables faster monitoring and allows more powerful and more dynamic reactions.

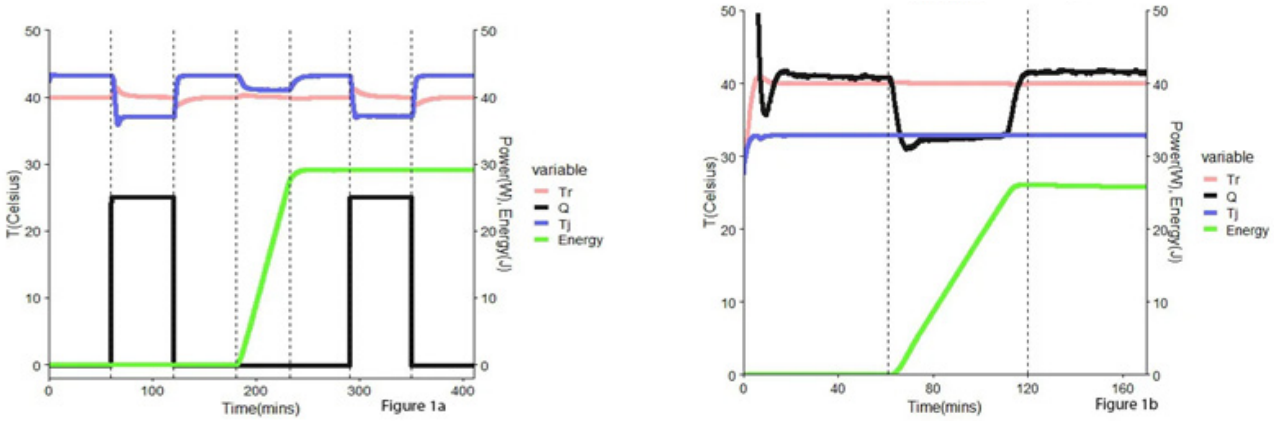


Figure 1. Comparison between Heat Flow (HF) – left – and Power Compensation (PC) – right – methodologies. Tr – reactor temperature (°C), Q – heater power (W), Tj – jacket temperature (°C), Energy (kJ)

Power Compensation and Heat Flow calorimetry methodologies have significant fundamental differences. However, there are no statistical differences in the reaction enthalpy measured by both methodologies. While Heat Flow calorimetry has long been established as the industry standard in calorimetry, Power Compensation offers the advantage of reducing process times and increasing process productivity.

Reflux Calorimetry

This technique is non-isothermal calorimetry and is used for calorimetry for reactions at the boiling point. This is available as an optional extra on the H.E.L's Simular system, speak to your sales representative for more information.

Configuration to meet your needs

Simular

- Single reactor vessel (250 mL to 5L)
- Atmospheric pressure
- Highly configurable
- A variety of probes and sensors, including temperature, pressure, pH, turbidity, and other sensors, are available

High Pressure Simular

- Single reactor vessel (250mL to 5L)
- Pressure up to 100bar (200bar reactor volume and material dependent)
- Comprehensive options for reaction control and monitoring

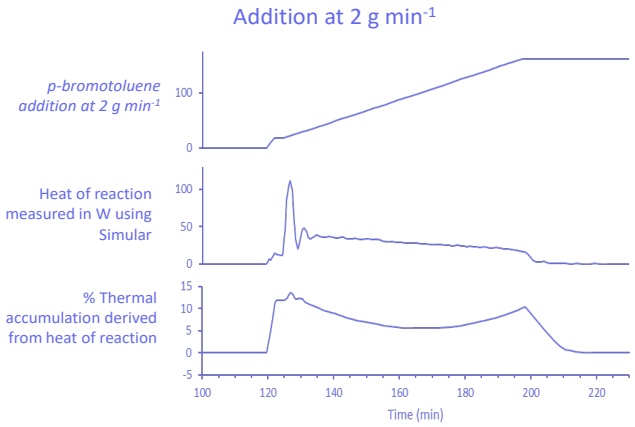
Dual Simular

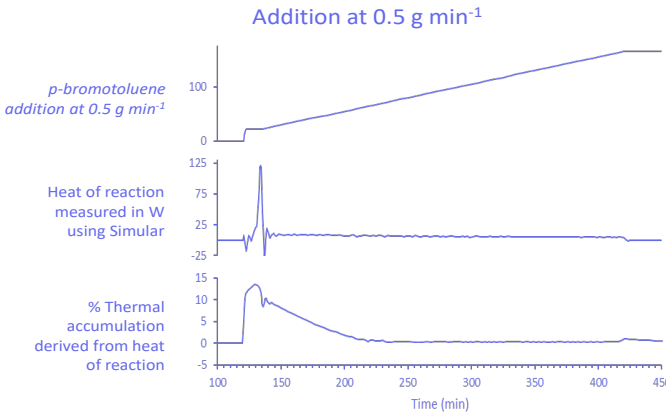
- Dual reactor vessels (250mL to 5L)
- Atmospheric pressure and high pressure (vacuum to 100bar, 200bar reactor volume and material dependent)
- Future-proof modular and upgradeable design

Case study

Grignard Reagent Synthesis

In this case study, H.E.L's Simular was used to evaluate risks and optimize the scale-up of a reaction involving p-bromotoluene. The heat of reaction was measured at different dosing rates to analyze thermal accumulation during the feed. Using Stoessel criticality, risks at various feed rates were quantified. The product yield was also assessed by gas chromatography (GC), ensuring both safety and efficiency in the process.





Dosing rate (g min^{-1})	Theoretical adiabatic temperature rise (°C)	Semi-batch MTSR (°C)	Risk level (derived from Stoessel criticality diagram)	Yield (wt%) (determined by GC)
2.0	204.87	79.41	Level 3, Potential hazard, risk-reducing measures must be implemented	95.71
1.0	191.53	71.20	Level 3, Potential hazard, risk-reducing measures must be implemented	92.15
0.5	177.34	59.79	Level 1, Process presents a low thermal risk – additional measures not required	87.39

In this study, the Simular was used to identify a feed rate that balances acceptable yield with minimal risk. A feed rate of 0.5 g min^{-1} achieved a risk level of 1 and a yield of 87.39%. Critical reaction parameters were established, providing greater confidence in the safe and profitable scale-up of the process.

Features and options

- Configurable system: dual reactor and pressure options
- Three modes: Calibration-free Power Compensation Calorimetry, Heat Flow Calorimetry or Reflux Calorimetry
- Versatility of use: Calorimeter or automated reactor
- Safety features: Minimize safety hazards and maximize product yield, real-time calorimetry software features

Specification point	Simular
Typical applications	• Process safety • Process scale-up • Process development and optimization
Vessel material	Glass, 316 Stainless steel, and Hastelloy C276
Vessel volume	250 mL to 5L*
Dual vessel	A dual vessel option is available (typically with a glass, ambient pressure vessel and a metal, high-pressure vessel) including a larger dual frame and switching between reactors
Temperature range	-80°C to 250°C (dependent on reactor material and circulator)*
Pressure range	Vacuum to 100 bar (optional pressure – up to 200 bar, depending on reactor volume and material)*
Sensor options	• Temperature, pressure, pH, turbidity, and other sensors are available • Integration of third-party probes is possible, such as in-situ FTIR, particle sizing probes, and Raman probes with software integration
Control & analysis software	• Easy to use, powerful software designed both advanced users and beginners • Intelligent automation: Customizable interface with real-time sensor readings, allowing for feedback loops, and reactor parameters based on user preferences • User-defined experiment plans covering simple to advanced reactions • Common software across H.E.L group process safety product range for ease of use and to save time on training
Calorimetry modes	Isothermal calorimetry: • Power compensation calorimetry • Heat flow calorimetry • Optional: Reflux calorimetry • Other methodologies: Isoperibolic calorimetry
Safety features	Automatic user-configurable shutdown procedures if a safety condition is exceeded to ensure user safety

* Contact your local H.E.L group representative to discuss additional options.

What our customers say...

“The ease of use of and the accuracy of the TSu and Simular systems, made my work much easier and accurate. I would like to mention the great relationship I established with the service engineers and the sales people at H.E.L. With their help I was able to customize the software and the hardware of the equipment to our specific needs.”

Theravance Inc – USA

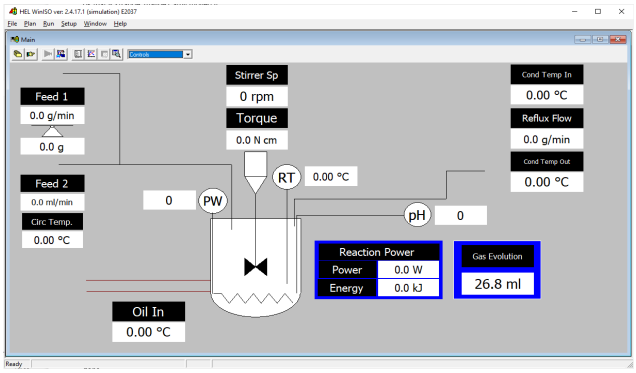
WinISO

Bringing effortless efficiency to your laboratory automation

With the power of WinISO, you can elevate your research with a software solution that adapts to your needs.

Flexibility and control

- Fully configurable workspace – improved efficiency by displaying the info you need
- No swapping between windows required; configure the workspace to suit you
- Powerful and flexible code base combined with an intuitive and user-friendly design



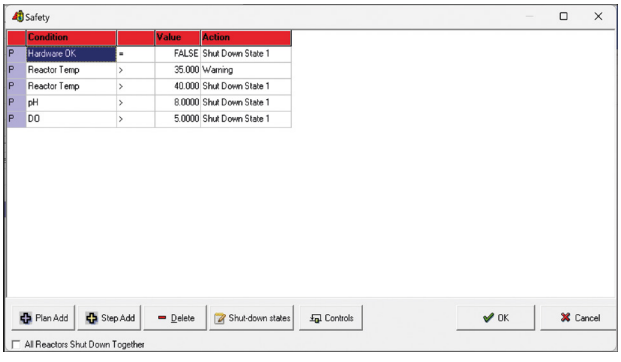
Empowering proactive experimentation

Designed around the user experience, WinISO combines:

- advanced real-time calorimetry features and data display
- automated monitoring of experiment completion and failure states
- rapid data capture modes across single or multiple reaction systems

Real-time interactivity

- Change and adapt on the fly as you navigate through your experiments
- Interactive design empowering real-time adjustments
- Ensure that your research evolves, aligning with your insights and discoveries



Safety at the core

- Robust safety features protect both the operator and the experiment
- Ensuring a secure environment for your experiments allows you to focus on pushing boundaries

Upgrades, Support and Training

We understand that your needs can change over time and you may require:

- A system upgrade
- Training for new team members
- Support on your processes
- To book some time with our service team

Our dedicated service team and highly knowledgeable technical staff will work with you to find the right solution.

Customer Service Enquiries & Techinical Support Requests

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About H.E.L Group

H.E.L Group's mission is to work together with chemistry, safety and biotechnology experts to engineer and unleash the full potential of the scientific community. To this end, H.E.L develops and manufactures innovative scientific instruments and software designed to optimize the efficiency, safety and productivity of key processes in chemistry and biology applications.

The H.E.L team includes highly skilled process and software engineers, based at their extensive research and manufacturing facilities in the UK, as well as sales and support offices around the world.

H.E.L has a long history of solving complex challenges for customers. For more than 30 years the company has worked with businesses and laboratories globally, providing proprietary automated solutions for the pharma, biotechnology, chemical, battery and petrochemical sectors.
H.E.L is accredited with ISO 9001 : 2015 and ISO 14001 : 2015.

- With a strong focus on the customer, our **service and support** enables our customers to keep working efficiently
- Our **wide range of customizable products** put the customer at the heart of what we do, with solutions designed around their needs

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