h.e.l

Chemical Synthesis

Automated reaction systems for chemical synthesis, process development & scale-up

www.helgroup.com

Offering you a complete range of chemical synthesis solutions

From identifying active molecules through to pilot-scale synthesis, H.E.L Group provides a comprehensive range of automated reaction systems to facilitate chemical research, development, optimization, and scale-up. In this brochure, we focus on solutions for chemical synthesis.

Chemical product development is typically characterized by three main stages:

- **Discovery**
- **Process development**
- **Scale-up prior to full manufacture**

At the **discovery** stage, including **lead optimization**, we provide solutions for small scale reactions, reagent screening and parallel synthesis. The benefits of using these are:

- **Increased productivity:** synthesis of multiple molecules and screening of multiple conditions using our parallel synthesis range
- **Space-saving:** compact parallel synthesis systems
- **Improved safety:** automated synthesis using our parallel synthesis range and hazard screening using our process safety range

We provide an even more comprehensive range of solutions for **process development** and **route optimization.** From **small-scale process development** and **Design of Experiment (DoE)** to **calorimetric studies**, our systems offer essential features, including:

- **Temperature control:** to study the effect of temperature and thermal events on reactions
- **Overhead stirring:** to apply the manufacturing conditions as early as possible in the development
- **Data recording and reproducibility:** our chemical synthesis systems are all **software-controlled.** The data collected enables the understanding of the chemical process, as well as technology transfer for scale-up
- **Multiple reactions:** using our parallel synthesis range, ideal for DoE
- **Safety:** minimize hazards and optimize reactions using our **reaction calorimetry** tools

Once the process has been defined at bench scale, our **scale-up** solutions offer similar benefits to our process development range, at **pilot scale**. These are ideal to perform **proof-of-concept** experiments before moving to manufacturing scale.

Your Needs

Our Solution

Discovery

Productivity, space, and safety
For small-scale reactions, reagents screening, parallel synthesis

Parallel Synthesis
PolyBLOCK & AutoMATE

Catalyst Screening
See High Pressure Catalysis portfolio

Hazard Screening
See Process Safety & Scale-up portfolio

Process Development

Temperature control, overhead stirring, data recording, reproducibility, and safety
From DoE to reaction calorimetry

Parallel Synthesis
PolyBLOCK & AutoMATE

Crystallization & Solubility Screening
See Crystallization portfolio

Bench-Scale Reactors
AutoLAB

Hazard Screening
See Process Safety & Scale-up portfolio

Reaction Calorimetry
Simular

Scale-Up

Mimic manufacturing conditions, reproducibility and safety
For pilot-scale reactions

Pilot-Scale Reactors
AutoLAB

Adiabatic Calorimetry
See Process Safety & Scale-up portfolio

Manufacture

Parallel Synthesis in Discovery

PolyBLOCK
AutoMATE

Building a library of potential candidate lead molecules with the desired characteristics (e.g., biological activity towards a target molecule) requires a targeted parallel synthesis approach, where the ability to run multiple experiments simultaneously dramatically improves productivity.

Similarly, the same approach can be applied for lead optimization – to improve efficacy or other parameters.

PolyBLOCK 8

AutoMATE

Parallel Synthesis

The **PolyBLOCK** and **AutoMATE** platforms are highly versatile automated parallel synthesis platforms. The **PolyBLOCK 4** and the **PolyBLOCK 8** support 4- and 8- independently controlled reactor zones. This compact configuration is designed for situations where bench space is limited. The **AutoMATE** supports 4 independently controlled reactor zones in a linear configuration and is ideally suited for more complex applications. These systems support a wide range of vessel options, from 2 ml vials to 500 ml vessels for the 4-zone versions.*

High Pressure Options

Both platform types use a modular design, enabling capabilities of the system to be easily expanded and adapted. They are also available in high pressure variants with stainless steel and Hastelloy reactor options, supporting the study of hydrogenations and other high-pressure reactions.

*Figures stated here are for standard configurations; please see our **Chemical Synthesis Specification Sheet** for more information on other options available.

Lead Optimization

The wide range of functionality, the number of reactor zones, and the large number of reactor options ensure the **PolyBLOCK** and **AutoMATE** platforms are especially well-suited for lead optimization campaigns. They enable the synthesis of candidate molecules, their modification, and subsequent screening to enable the selection of the most promising molecule for further development.

Hazard Evaluation

Safety considerations are also important when exploring candidate molecules. H.E.L Group has a wide range of solutions within process safety, including hazard screening tools – please see our **Process Safety and Scale-up** portfolio for further details.

Bespoke Solutions

H.E.L Group has a well-established history of developing tailored, automated reactor solutions for the chemical and pharmaceutical industries. If you are interested in a customized solution, please **contact us** to discuss your specific requirements.

Parallel Synthesis in Process Development

PolyBLOCK
AutoMATE

Optimize reaction parameters in parallel. Reduce process development time with controlled conditions for meaningful and reproducible results, while recording data for a better understanding of reactions.

PolyBLOCK 4

AutoMATE

Selecting the Best Synthetic Approach

The **PolyBLOCK** and **AutoMATE** platforms enable multiple synthetic routes to be investigated in parallel, identifying the optimal conditions to take through to scale-up. Conversion efficiency, economic viability and potential scale-up challenges can be identified at this stage.

The **PolyBLOCK** and **AutoMATE** platforms offer essential features for early process development in a compact footprint:

- Temperature control from ambient to 200 °C with potential for additional cooling to achieve sub-ambient temperatures
- Option for overhead stirring to mimic manufacturing as early as possible in the development process
- Recording and analysis of data to understand the reactions before scale-up
- Many other add-on options, such as controlled additions (liquid and gas), reactions under pressure and turbidity measurements

Design of Experiment (DoE)

Identifying the critical parameters of a process is crucial for maximizing the output (e.g., yield, purity, selectivity). These parameters can be explored in DoE campaigns using the independent reactor zones of the **PolyBLOCK** and **AutoMATE** platforms.
The **PolyBLOCK 4** and the **PolyBLOCK 8** are compact, parallel synthesis platforms, ideal for limited bench space, supporting 4- and 8- reactor zones, respectively.
The **AutoMATE** is a linear, 4-zone parallel synthesis platform, designed for more complex applications. These systems support a wide range of vessel options, from vials to 500 ml vessels for the 4-zone versions.*

*Figures stated here are for standard configurations; please see our **Chemical Synthesis Specification Sheet** for more information on other options available.

High-Pressure Reactions

High-pressure variants of the **PolyBLOCK** and **AutoMATE** platforms are also available for reactions up to 200 bar. These are ideal for applications such as high-pressure catalysis.

Batch vs Continuous flow

Comparing batch synthesis with continuous flow methods can be valuable for process optimization. Using the **FlowCAT**, alongside the parallel reactor platforms can help determine which method is best for optimal conversion and hazard mitigation.

H.E.L Group offers a wide range of dedicated solutions in catalysis screening and process optimization – please see our **Catalysis** portfolio for more information.

Crystallization Studies

With H.E.L's proprietary turbidity sensors, the **PolyBLOCK** and **AutoMATE** platforms can be configured for real-time crystallization studies. Further data analysis allows for the characterization of metastable zone width (MSZW), providing valuable information for further process development and scale-up.

Please see our **Crystallization** portfolio for our full range of dedicated solutions to crystallization and solubility monitoring.

Safety

Safety is also an important consideration when assessing different synthetic approaches. H.E.L Group has a wide range of solutions within process safety, including hazard screening tools – please see our **Process Safety and Scale-up** portfolio for further details.

Bespoke Solutions

H.E.L Group has a well-established history of developing tailored, automated reactor solutions for the chemical and pharmaceutical industries. If you are interested in a customized solution, please **contact us** to discuss your specific requirements.

Reaction Calorimetry in Process Development

Simular

Understand the thermodynamics and kinetics of your process under isothermal or non-isothermal conditions for safe scale-up. Reaction calorimetry provides data to enable the safe running of chemical processes.

Simular (Glass Reactor)

Simular (Metal Reactor)

Optimizing Reactions for Scalability and Safety

The **Simular** is a reaction calorimeter designed to investigate the thermal properties of a chemical reaction under the intended operating conditions. The thermodynamic and kinetic information obtained can be used for the optimization of process conditions for maximized conversion while minimizing safety hazards.

Isothermal calorimetry

The **Simular**, can be operated in two isothermal modes:

- the well known heat flow method
- the H.E.L method of power compensation, which is very responsive

Non-isothermal calorimetry

The **Simular** can also be operated in two non-isothermal modes: ramped and reflux, for more specific applications.

Mitigating thermal hazards

The **Simular**, alongside the **Phi-TEC I** and the **Phi-TEC II**, can also be used to help identify the operating conditions required to minimize safety risks. Please see our **Process Safety & Scale-Up** portfolio for more information on our hazard screening solutions and how reaction calorimetry can be applied to process safety.

Configurable Design

The **Simular** is a flexible platform that can be adapted to suit individual needs (e.g., dual-reactor capability, high and low pressure options). Please **contact us** to discuss your specific requirements.

Automated Reactors in Process Development and Scale-Up

AutoLAB

Scaling up a chemical process safely and efficiently requires a deep understanding of how the reaction will behave in larger volumes. This knowledge is critical to optimizing operating conditions while mitigating any thermal and pressure hazards.

Optimization for Scale

Jacketed reactors can replicate manufacturing operations at the laboratory scale, enabling the efficiency of the desired reaction to be evaluated under representative conditions. Reaction rate, yield, and selectivity can be assessed, and the information generated can be used to inform further optimization studies.

The **AutoLAB** is a highly configurable automated laboratory reaction system, supporting vessel sizes ranging from 1 L (bench-top) to 20 L (floor standing frame).* It is also available as a high-pressure variant, facilitating the study of reactions operated at pressure, and enabling the replication of the pressure effects found at a manufacturing scale.

By closely mimicking production scale conditions at the bench to pilot scale, it is possible to improve the efficiency of the process prior to costly scale-up. The **AutoLAB** supports optimization of reaction efficiency by enabling the study of factors such as the stirrer design, addition rate, mixing regime, and other operating conditions. Being software controlled, the **AutoLAB** minimizes human error - experiments are reproducible, and the data recorded can be used for further scaling up.

Mitigating Worst-Case Scenarios

Scaling up a process requires accurate knowledge of any potential exothermic events so that appropriate safety measures can be implemented. Please see our **Process Safety & Scale-Up** portfolio for more information.

Bespoke Solutions

H.E.L Group has a well-established history of developing tailored, automated reactor solutions for the chemical and pharmaceutical industries. If you are interested in a customised solution, please **contact us** to discuss your specific requirements.

*Figures stated here are for standard configurations; please see our **Chemical Synthesis Specification Sheet** for more information on other options available.

labCONSOL®

Bringing effortless efficiency to your laboratory automation

Built around the next generation of the proven WinISO software engine and introduces new features that enable scientists to improve laboratory efficiency and boost productivity.

Designed around the user experience, labCONSOL® combines:

- **advanced real-time data display**
- **automated monitoring of experiment completion and failure states**
- **rapid data capture modes**

across single or multiple parallel reaction systems.

Enabling researchers to quickly and accurately track how an experiment is proceeding, focusing on the most critical aspects, avoiding unnecessary repeated lab work, which can be both costly and time-consuming.

Better user experience – increased productivity

- New intuitive design means less training time required
- Creating new plans/recipes is now simplified. labCONSOL® will also provide hints and tips along the way to prevent errors.
- New plans can be created while an existing experiment is running

Fully configurable workspace – improved efficiency by displaying the info you need

- No swapping between windows required; configure the workspace to suit you.

Improved data-logging and graphing functionality

- New SQL database for file management – no risk of data loss from any experiment
- Improved graphing performance – view entire experiment on a single graph

Invest for the future – benefit from additional features and functionality

- Free software upgrades during the warranty period of your equipment
- Can be extended with a Premium Agreement or Extended Warranty

Powerful software

- One piece of software to support the full range of H.E.L equipment
- Powerful and flexible code base combined with intuitive and user-friendly design

For more information, and how to request an upgrade, visit https://helgroup.com/products/labconsol/ or speak to your local H.E.L representative

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 & Technical 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

H.E.L Group

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