

Chem-SCAN

HIGH PRESSURE

A POWERFUL TOOL FOR PROCESS DEVELOPMENT CHEMISTS

The HP Chem-SCAN is a parallel reaction system designed for the rapid screening of high pressure reactions and heterogeneous catalysis systems.



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Chem-SCAN



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HIGH PRESSURE Chem-SCAN

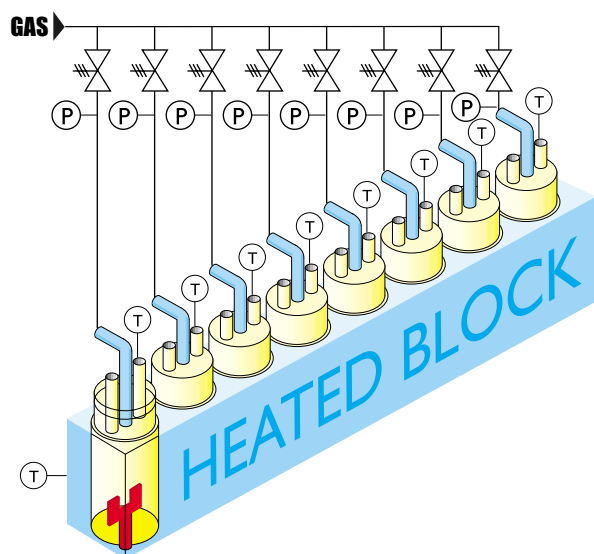
The High Pressure Chem-SCAN is a parallel reactor system designed for the rapid screening of high pressure reactions and catalysts.

The system consists of a block with eight high pressure reactors, all aggressively stirred. These are connected to a gas dosing manifold that allows independent controlled addition of gas to a pre-set pressure.

Capabilities

The system allows simultaneous study of several high pressure reactions with reactor volumes of 10 or 15ml.

The unit is capable of operating up to 100 bar (1500psi), with a standard temperature range of ambient to 200°C and there are also both low and high temperature options. The system is equipped with aggressive high torque magnetically coupled agitation of up to 1500 rpm.



- ▲ Hastelloy reactor versions for corrosive gases/liquids.
- ▲ Dual-temperature jacket for investigating the effect of temperature.
- ▲ Range of pressures investigated in a simple run.
- ▲ Fully software controlled with complete data logging.
- ▲ Experimental recipes available for user editing.
- ▲ Remote liquid addition for thermally sensitive catalyst; air sensitive chemicals also handled.
- ▲ Operation up to 100 bar (1500psi)
- ▲ Live display of gas uptake





Pressure control

Pressure difference between reactors in a single run can be up to 30 bar (450psi). The variation in pressure in a given reactor depends on the difference between the set point and the feed gas pressure. Fluctuations of less than 0.2 bar can be achieved.

Sensitivity

The presence of a reaction is detected by a fall in gas pressure in each reactor, thus defining the sensitivity.

For units set up to run at 100 bar, pressure reduction of around 0.1 bar (0.05 mmoles of gas) can be detected.

High pressure liquid addition

The Chem-SCAN has a high pressure liquid feed option, which is fully automated, up to pressures of 100 bar (1500 psi), with an accuracy of around 0.05ml or better. If necessary, such additions can be performed at a predefined rate – representing for example a semi-batch reactor.

Aggressive Chemistries

The system is available with all wetted parts in Hastelloy to enable the study of even the most aggressive of chemistries. In addition glass inserts are available, as are a range of agitator materials to enable the study of chemistry under the optimal operating conditions.

Controlling Software

The key to the system is the highly flexible and user friendly modular software, developed along the lines of our universally acclaimed winISO.

Reactors can be run at different pressures and the rate of gas uptake (semi-quantitatively) is calculated

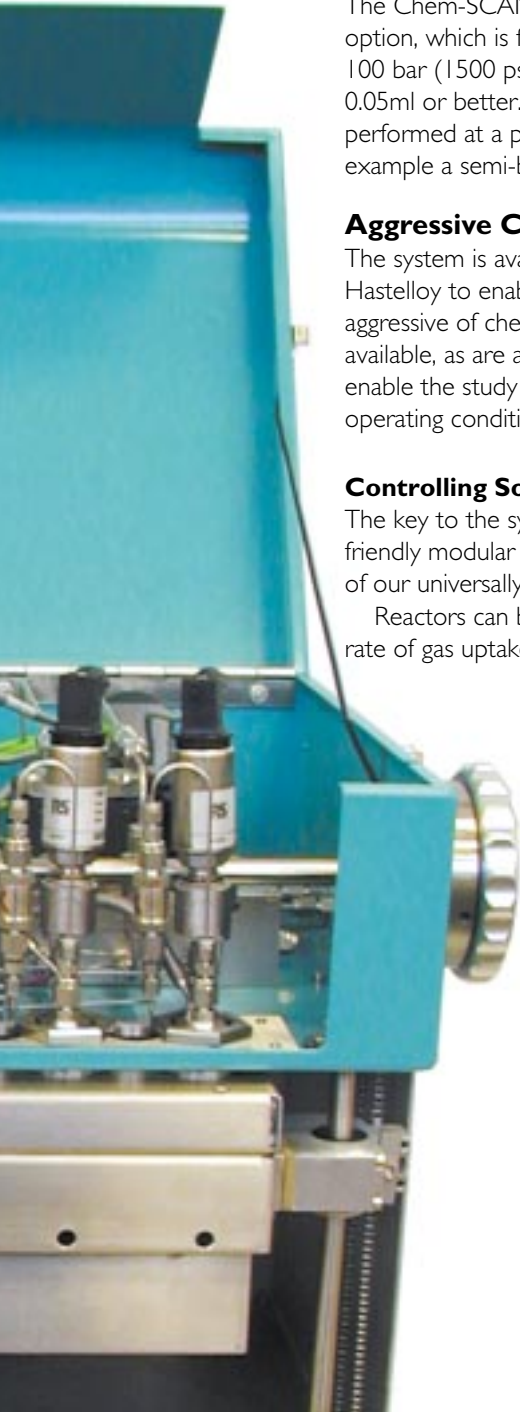


on line. The system is totally computer controlled.

The underlying winISO software is fully able to cope with all variations of experiments but "standard" experiments can be run simply by completing an input form.

The system is configured to allow easy selection of the test sequence, typically:

- ▲ Inert gas purge with choice of pressure and repeat steps
- ▲ Reactive gas purge with choice of pressure and repeat steps
- ▲ Selection of reactive gas and then choice of operating pressures for each reactor
- ▲ Termination of gas feed determined by rate of reaction falling below a user-defined threshold, or after a certain time has elapsed.
- ▲ Final inert gas purges
- ▲ Inert gas purging and related procedures are automatically performed
- ▲ Stirrers can be programmed to turn on or off at any time whilst speed can also be adjusted



MULTIPLE REACTORS WITH SCALABLE DATA

auto-MATE^{HP} is the high pressure version of the market leading process optimisation tool auto-MATETM.

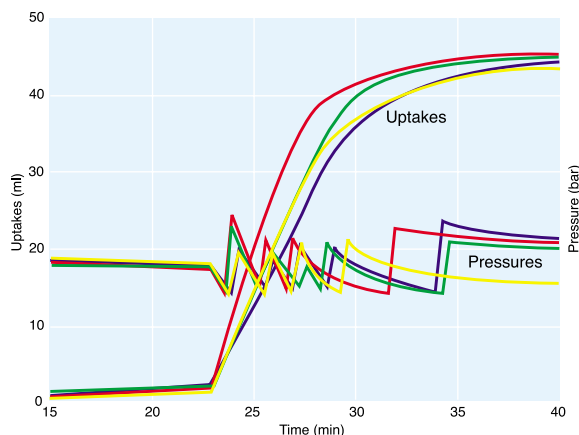
This fully computer controlled system consists of reactors of between 50ml and 100 ml volume and generates scalable data in continuous, batch and semi-batch chemistries.

The auto-MATE is highly configurable to meet the specific requirements of complex processes

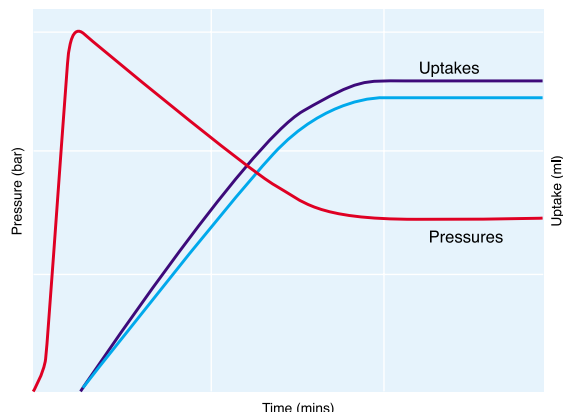


Applications: Hydrogenation catalyst screening

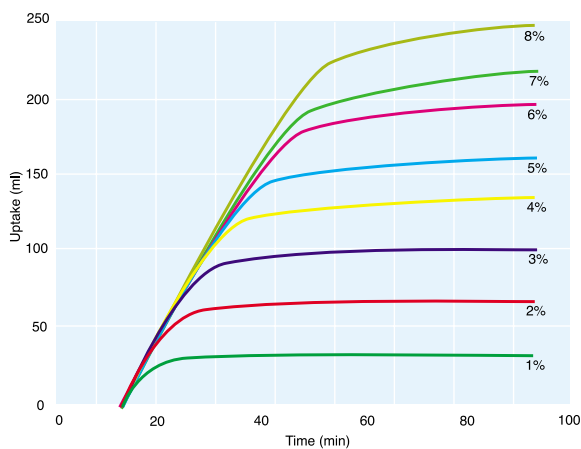
This is a typical trace of the data during a run. The pressure in each reactor falls as gas is consumed and this information is used to calculate the consumption. At a predetermined pressure, the reactor is "topped up" with fresh gas and this cycling continues until the pressure remains constant.



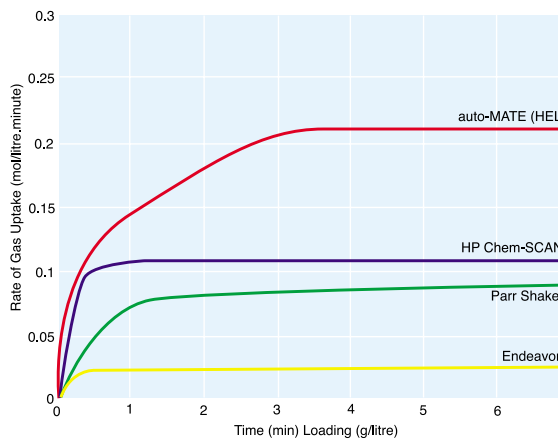
This is a very simple way to run the experiment. The reactors are charged to a pre-set pressure and the agitation is then turned on, to begin the reaction. Ideally suited to very fast reactions and it can highlight subtle differences very easily.



A set of 8 reactions, using different amounts of the same reagent at a fixed pressure. This is a good check for consistency and reproducibility. The plot shows data reported live at the end of a run.



This is a plot of data from many experiments showing the rate of initial hydrogen uptake as a function of catalyst loading. As can be seen, by data generated by Pfizer Inc (AIChE symposium 2002), the HP Chem-SCAN performs much better than competing devices in terms of the mass transfer limit.



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