



THALESNano

"Good reactions"™



H-Cube®

Next Generation Hydrogenation

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FEATURES

The H-Cube® represents the first in a new wave of continuous flow hydrogenation reactors. Utilizing water electrolysis to generate hydrogen, a catalyst cartridge system (CatCart®), and a continuous flow mechanism, H-Cube® makes hydrogenation safer, more efficient, and easier to perform.

- A continuous flow of substrate is combined with hydrogen, generated in-situ from the electrolysis of water
- The hydrogen/substrate mixture can be heated and pressurized up to 100°C and 100 bar (1450 psi) respectively
- The mixture is then passed through a packed catalyst cartridge (CatCart®), where the reaction takes place

Within 2 minutes, product emerges for fast reduction and optimization. Reductions varying in scale from 10 mg-100 g can be performed on the same compact reactor.

H-Cube® is capable of hydrogenating a wide range of different functional groups, for example:

- Nitro reductions
- Alkene and alkyne saturation
- N- and O-debenzylations
- Nitrile reductions
- Heterocycle saturation
- Imine reduction
- Desulfurization
- Dehalogenation

Catalyst selection or varying the amount of hydrogen produced on the H-Cube® can be used to perform selective reductions.

ADVANTAGES

Safer

- No gas cylinders or other external hydrogen source
- No catalyst filtration or direct catalyst handling
- Easy catalyst exchange

Efficient

- Analyze reaction results after 2 minutes
- Perform up to 50 different validation conditions in a day
- Higher reaction rates with increased phase mixing
- Easy to use, touch screen controlled

Convenient

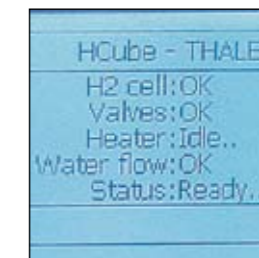
- Compact size can be used in a standard laboratory fume hood
- No special training or skills required to operate
- Can be coupled to standard liquid-handling robots for the integration of hydrogenation into an automated synthesis process

PRODUCT UPDATE

The H-Cube® is now also available with stainless-steel reaction line. The new steel reaction line allows the H-Cube® to be used with a wider range of solvents which the standard PEEK reaction lines don't tolerate.



"Good reactions"™



1. Touch screen panel

Every operational step of the H-Cube® is conveniently controlled using a touch screen panel. Parameters such as temperature, pressure, hydrogen production, and flow-rate can be adjusted through the screen, providing simple and rapid reaction set-up, system monitoring, and reaction control.



2. Solvent/Substrate inlet

The solvent/substrate is introduced into the reactor at a steady flow via an external HPLC pump.



3. Heating unit

The heating unit heats both the reaction line and the catalyst cartridge (CatCart®) up to temperatures of 100°C. The low volumes of substrate and hydrogen mean that heating is quick and efficient, while easy to monitor and control.



4. ThalesNano's CatCart®

ThalesNano's CatCart® are sealed cartridges containing heterogeneous catalysts for use with the H-Cube®. Exposure to the catalyst is limited by removing the need for filtration. The cartridges are easy to install and dispose of, and significantly increase the ratio of the catalyst to the hydrogen and substrate, which in turn increases the reaction rate.



5. Product collector

The reaction mixture or product collects in the collection vial. The short reaction time (in most cases a few minutes) means that analytical samples can be taken to measure product conversion and any necessary system adjustments (temperature, pressure, flow-rate, or catalyst) made immediately to optimize the reaction.



ThalesNano's CatCarts®

Thales' CatCarts® contain sealed heterogeneous catalysts, which can be used in hydrogenation and other heterogeneously catalyzed reactions in the H-Cube®. Exposure to the catalyst is limited by removing the need for filtration, while the cartridges are easy to install and replace. In the CatCarts®, the ratio of catalyst to hydrogen and substrate is significantly increased, which results in faster reaction rates.

CatCarts® come in three standard sizes (30, 55, 70 mm). The smallest CatCarts® are used typically to reduce up to 1g of substrate, while the longest CatCarts® can reduce up to 100 g of material in a day with no signs of catalyst deactivation.

If you require further information on the instrument, or would like to have a Demonstration scheduled, please contact:

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The following CatCarts® are currently available:

- 10% Pd/C
- Inert CatCart®: Quartz
- Inert CatCart®: Titanium
- (2,5% Pt 2,5% Pd)/C
- Raney-Ni
- 10% Pt/C
- 5% Rh/C
- 20% Pd (OH)₂/C (Pearlmann's catalyst)
- Raney Cobalt
- Raney Copper
- 5% Pd/Al₂O₃
- 5% Pd/C
- 5% Ru/Al₂O₃
- 5% Pt/Al₂O₃
- 5% Pd on CaCO₃ / Pb (Lindlar's catalyst)
- 5% Ru/C
- 5% Re/C
- 5% Pt/C, Sulfided
- 5% Rh/Al₂O₃
- PtO₂ (Adam's Catalyst)
- Pricat Ni 55/5P
- NP Pd(0)EnCat™ 30 *
- 5% Pd/BaSO₄
- Nickel sponge, promoted 1% Mo
- (5% Pd, 1% Fe)/C
- (4,5% Ru, 0,5% Pd)/C
- 1% Pd/Al₂O₃
- 10% Pd/Al₂O₃
- Pd/C- Ethylenediamine
- 1% Ir/C
- Ni/Si-Al
- 5% Pd/SiO₂
- 1% Pd/C
- 2% Pd/SrCO₃
- 1% Pt/Al₂O₃
- PdO
- Pd black
- [{RuCl₂(mtpms)₂}]₂
- Wilkinson's Catalyst Rh(I)(TPP)₃Cl polymer bound
- PdEnCat™ 30 *
- PdEnCat™ TPP30 *, **
- Pd(II)EnCat™ BINAP 30 *, **
- Tetrakis (TPP)-palladium polymer bound
- Pd(II)EnCat™ TOTP 30 *
- RuO₂
- IrO₂
- Fibrecat 1001
- Fibrecat 1007
- Fibrecat 2003
- Fibrecat 2006
- 1% Pt/C
- 5% Ir/CaCO₃
- 5% Pt/C

The list of available CatCarts® is being constantly updated with new catalysts. In addition, Thales Nanotechnology will make CatCarts® to order.

* Encat is a trademark of Reaxa Ltd.

** Pd Encat technology, international patents have been applied for, including PCT/GB 02/03135.