Can I transfer any reaction in solution from batch to flow?

In theory, yes, you can pump any homogeneous solution through a fixed-bed in the H-Cube Pro. However, the H-Cube Pro was designed for heterogeneous hydrogenation reactions. Other reactions which require heterogeneous gas/liquid/solid conditions with short reaction times (less than a minute) might proceed well on the H-Cube Pro. For homogeneous reactions that require a longer reaction time, other instruments such as the Phoenix Flow Reactor would fit better (residence time ranges from ca. 10 to 120 min).

Can I use the H-Cube Pro to perform deuterated reactions only? Would it have any negative impact on the electrodes?

Yes, you can use the H-Cube Pro and the Mini Plus for performing deuterations. Make sure that the highest quality D_2O is used (same specifications should apply as for H_2O).

Can the Phoenix Flow Reactor do the same reactions as the H-cube Pro?

The Phoenix Flow Reactor does not have an in-built hydrogen generator. You need to connect it to either the H-Genie, the H-Cube Pro or an H_2 cylinder to be able to perform hydrogenations with H_2 gas. Apart from this limitation, you can fit the same cartridges to the Phoenix (30 and 70 mm long CatCarts) that are used in the H-Cube Pro.

What is the total reaction time?

It depends on the flowrate you set and total volume of your tubing (dead volume). To find out the total process time, from the starting materials solution to the collection flask, you then need to divide the total dead volume by the flowrate. Nevertheless, and as an estimation, the residence time can range from ca. 2 to 40 seconds depending on the conditions (catalyst, CatCart size, flowrate etc).

What is the maximum concentration of reactants that can be used?

The typical concentration range is between 0.05 and 0.1 M. However, sometimes higher concentrations even up to 0.5 M are achievable. Please note that the highest operating concentration will depend on all other reaction conditions (e.g. solubility of the substrate, catalyst, reaction time etc.).

What is the quantity of catalyst in the 30 & 70 mm CatCarts?

It varies from a catalyst to another. A 30 mm Pd/C CatCart will contain 150±5 mg of Pd/C while a 70 mm will contain 400±5 mg of Pd/C. For comparison, A 30 mm Raney Nickel CatCart will contain 490±5 mg of Raney Nickel and a 70 mm will contain 1660±5 mg of Raney Nickel.

Can I repack the cartridge by myself?

Yes, with the CatCart Packer, you can fill cartridges with your own catalysts.

Nevertheless, we do not recommend refilling due to the chance of cross contamination and possible damage of the sealing, and use new cartridges instead.

Can I reactivate the catalyst?

It is possible in cases of inhibition, not possible in cases of poisoning. For example, if the product is an amine, that inhibited the Pd or Pt type catalysts, the activity can be recovered by washing it with MeOH or THF. For Raney Nickel, washing with it with water at high temperature and pressure under H_2 can enhance the activity, and also works as reactivation.

What is life cycle of cartridge or in another words, how many mg-s or moles of a sample can I reduce with the CatCarts?

The catalyst activity will depend on the reaction and materials, as some will poison the catalyst. For some materials, you will only be able to reduce let us say 50 mg of compounds but in some instances, you could reduce grams of the same substrate. As a general example, thiols and other sulphur-containing compounds tend to poison transition metal catalysts.

How can I check the catalyst activity?

You need to monitor the conversion of your product time-to-time. There is no direct way to analyse the catalyst inside the CatCart.

Can one measure the hydrogen consumption?

Unfortunately, we cannot measure the hydrogen consumption.

If one electrode is faulty, can the instrument still generate hydrogen?

Yes, the instrument can still build up the pressure of Hydrogen even with one cell.

Can I analyse my reaction with TLC plate monitoring?

Yes, you can monitor the advancement of your reaction with TLC plate monitoring the exact same way you would do it for batch chemistry by taking capillary tube samples from your collection flask(s).

How is the temperature controlled?

The temperature is controlled in the heater block, where temperature sensors, and therefore 3 temperature displayed: pre-heater, heater and post-heater.

When do I have to replace the water from tank? If I keep water for longer time can it damage my electrodes?

We recommend to replace the water with new milli-Q water weekly. The maximum conductivity of water is 71nS/cm (which correspond to a resistance of 14MΩ cm). Using lower quality water could cause irreparable damage of the instrument. If the instrument rests for a couple of weeks, a water tank purge with fresh water should be started before any work to clean the area around the cell membranes too.

Is there any alert if the hydrogen pressure increases suddenly due to the instrument error?

If for any reason, the H_2 pressure increases abnormally and reaches 140 bar, an error message appears and an emergency shutdown is initiated to empty the system.

What are the safety features during reaction in system?

A transparent plastic cover on the front, protecting the user from any, even unlikely, hazards, like tubing coming off.

All parts are in stainless steel, which can bear more higher pressure than the operating pressure, which makes the system inherently safe.

Catalyst is sealed in the cartridge, safe handling of pyrophoric, no spillage and no need for filtration

Only a minimum amount of hydrogen is store at a time inside the system.

What are the best advices for an optimal longevity of the system?

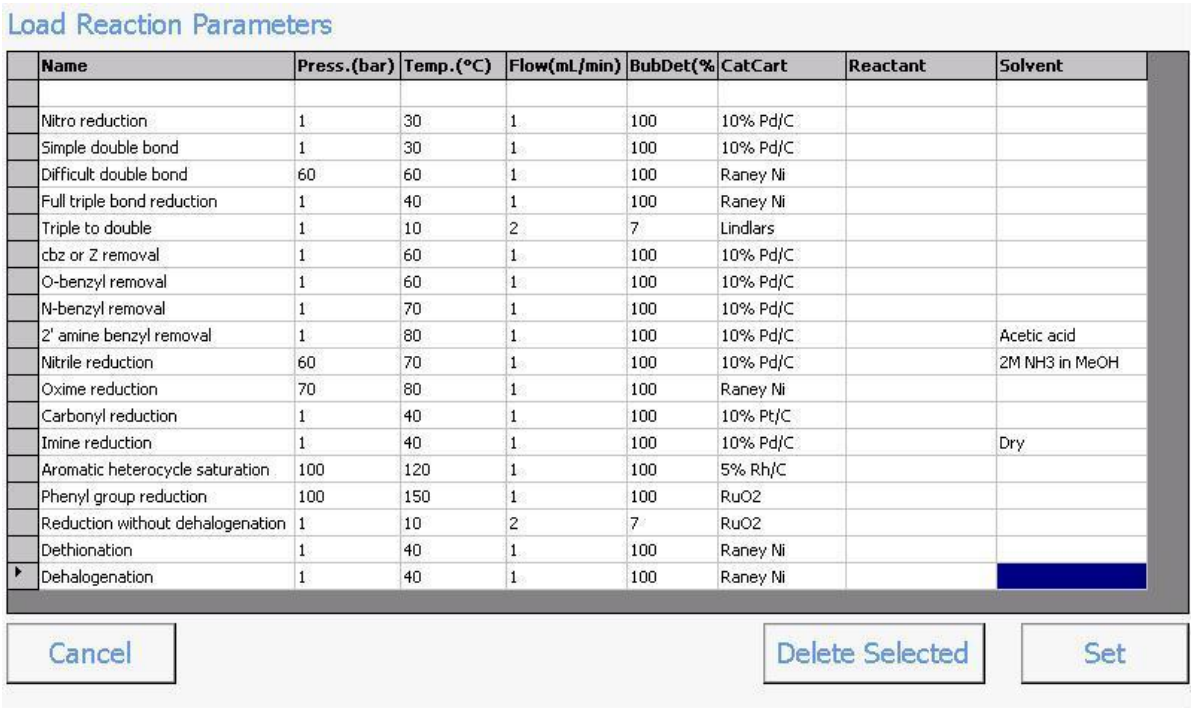
Keep the water in the water tank clean.

Wash the reaction line through after using it with clean solvent. Make sure to only use solvents, reagents compatible with the system. We have a compatibility list of solvents with the different materials (316L Stainless Steel, PEEK and PTFE). Most of the parts of the H-Cube Pro are made of 316L Stainless Steel

Be gentle with the screws as they have to be finger-tightened or only slightly more.

What is the flowrate that would give the best results?

It depends on a lot of factors, such as the concentration of the reagent solution and the synthetic transformation to be performed. We have a quick start reaction guide that advises some good starting conditions investigated and you can also find them uploaded and pre-set in the H-Cube Pro system software.



Name	Press.(bar)	Temp.(°C)	Flow(mL/min)	BubDet(%	CatCart	Reactant	Solvent
Nitro reduction	1	30	1	100	10% Pd/C		
Simple double bond	1	30	1	100	10% Pd/C		
Difficult double bond	60	60	1	100	Raney Ni		
Full triple bond reduction	1	40	1	100	Raney Ni		
Triple to double	1	10	2	7	Lindlars		
cbz or Z removal	1	60	1	100	10% Pd/C		
O-benzyl removal	1	60	1	100	10% Pd/C		
N-benzyl removal	1	70	1	100	10% Pd/C		
2' amine benzyl removal	1	80	1	100	10% Pd/C		Acetic acid
Nitrile reduction	60	70	1	100	10% Pd/C		2M NH3 in MeOH
Oxime reduction	70	80	1	100	Raney Ni		
Carbonyl reduction	1	40	1	100	10% Pt/C		
Imine reduction	1	40	1	100	10% Pd/C		Dry
Aromatic heterocycle saturation	100	120	1	100	5% Rh/C		
Phenyl group reduction	100	150	1	100	RuO2		
Reduction without dehalogenation	1	10	2	7	RuO2		
Dethionation	1	40	1	100	Raney Ni		
Dehalogenation	1	40	1	100	Raney Ni		

Can the software be upgraded online?

Usually, there is no need to upgrade the software. But in special cases, this would be done by our service colleague during a service visit.

What are the outputs for data transfer?

You can use a USB stick. We also have a solution to use the instrument using TCP/IP Protocol.

Can the H-Cube Pro be controlled by an external PC?

The instrument can be controlled from a distance via a TCP/IP protocol.

Can you run a future demo with the Phoenix Flow Reactor connected to H-Cube Pro to run reactions in series? Can the Phoenix Flow Reactor and the H-Cube pro be controlled and run in combination by a Control system / software?

Yes, we will run other webinars in the near future. This was just the part 1 of reactions performed with the H-Cube Pro (both alone or in combination with other module like Phoenix, gas module…).

The Phoenix Flow Reactor can be connected to the H-Cube Pro and controlled directly via the interface of the H-Cube Pro.