# Heterogeneous Catalytic Hydrogenation

## A New Two Day Course

16 - 17 April 2012

The Radisson Blu EU Hotel, Brussels, Belgium

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## Introduction

**Heterogeneous catalytic hydrogenation is of significant importance for the production of pharmaceuticals, nutraceuticals, flavours and fragrances, agrochemicals and fine chemicals.**

Indeed, an average of approximately 10% of all chemical steps in the production of such chemicals are catalytic hydrogenations. However, due to the multidisciplinary nature of heterogeneous catalytic hydrogenation, this technology is frequently improperly or inadequately used, which results in problems during scale up and negatively affects the economy of chemical processes and the quality of products.

Participants on this comprehensive course will be familiarized with all the important aspects of heterogeneous catalytic hydrogenation. Attendees will learn how to successfully design, develop and realize economic, safe, foolproof and ecological hydrogenation processes.

The main focus will particularly be on a deeper understanding of the underlying disciplines such as catalysis on surfaces and transport processes.

Guidelines on how to approach specific hydrogenation problems and concepts and tools for the design, development and scale up of catalytic hydrogenation processes will be presented, rather than summing up transformations of functional groups by catalytic hydrogenation, as this information can nowadays easily be searched and found in literature and patents.

## The course covers:

- Surfaces and metal surfaces
- Theory of catalysis on surfaces
- Transport steps and chemical steps in heterogeneous catalysis
- Kinetics (micro- and macrokinetics)
- Influence of variables (overview)
- Hydrogen sources (molecular hydrogen, hydrogen transfer agents, hydrogen solubilities)
- Hydrogenation catalysts (catalyst types, catalyst preparation, catalyst properties, catalyst activation and deactivation)
- Influence of solvents
- Influence of acids, bases, additives, modifiers
- Influence of substrates
- Influence of reaction conditions (concentrations, temperature, agitation)
- Chemical group transformations
- Reaction engineering aspects: suspension and fixed bed reactors; batch, semibatch and continuous operation modes
- Tools and guidelines for selection of chemical systems, determination of basic reaction data and successful scale up from laboratory to plant
- Economic aspects
- Safety aspects
- Analysis of surfaces and catalysts
- Rules of thumb, pitfalls

*Case Studies and Problem Sessions will be included throughout the course.*

## Course Outline

**Day One:**

Session 1: Physicochemical properties of surfaces.

Session 2: Metal surfaces, adsorption on surfaces

Session 3: Catalysis on surfaces, side reactions along with hydrogenations

Session 4: Transport steps and chemical steps in heterogeneous catalysis

Session 5: Kinetics

Session 6: Thermodynamics

Session 7: Variables (overview)

Session 8: Hydrogen

Session 9: Catalysts

**Day Two:**

Session 10: Solvents

Session 11: Acids, bases, additives, modifiers

Session 12: Substrates

Session 13: Influence of reaction conditions (concentrations, temperature, agitation)

Session 14: Chemical group transformations

Session 15: Reaction engineering aspects

Session 16: Tools and guidelines

Session 17: Economical aspects

Session 18: Safety

Session 19: Analysis of surfaces and catalysts

Session 20: Rules of thumb, pitfalls

## Fee & General Information

£1075.00

Includes lunch & refreshments, course dinner and comprehensive course manual.

The two-day course begins with registration at 8.45am on Monday 16 April and finishes at approximately 4.30pm on Tuesday 17 April.

Register for this course by using the form overleaf or call:

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## Course Tutor

**Felix Roessler** studied chemistry at the University of Zürich (UZH), Switzerland. After obtaining his PhD at UZH, he moved to Cambridge (GB) to work on organosilicon chemistry with Ian Fleming. He started his industrial career with Roche in Basel in 1980, first with central research where his focus was heterogeneous catalysis for the production of pharmaceuticals and fine chemicals and where he invented and developed an in-house high throughput screening system, particularly for investigating chemical reactions under elevated pressure/temperature conditions on a small scale, 10 years ahead of the emergence of commercially available systems. Next step was process research and development within Roche's pharma division, supporting medicinal chemistry, development and production regarding heterogeneous catalytic reactions. In 2000 Felix joined the vitamins division of Roche, where he initiated, developed and introduced highly economic and ecological heterogeneous catalytic processes for the production of nutraceuticals. Along with the take over of Roche vitamins by DSM in 2004, Felix worked as catalysis expert for DSM where he supported catalysis for the nutraceutical, pharma and base chemical divisions.

Felix was honoured twice with the Sandmeyer award in 1997 and 2008, granted by the Swiss Chemical Society. He is author of 18 publications, co-author of monographs and holds 4 patents.

Since his retirement in 2007, Felix is active as an independent consultant for all aspects of heterogeneous catalytic processes, from consulting regarding selection of the proper equipment, consulting regarding the selection of appropriate chemical systems and determination of basic reaction data, trouble shooting along with production processes, analysis of production processes regarding potential for improvements, to consulting and coaching R&D-chemists in the development of highly economic processes and successful scale up directly from laboratory to plant.

Felix Roessler can be contacted by email at:
**felix.roessler@gmx.ch**

## Venue

**Radisson Blu EU Hotel,** Rue d'Idalie 35, B-1050 Brussels, Belgium
Telephone: +32 2 626 81 11
www.radissonblu.com/euhotel-brussels

The Radisson Blu EU Hotel offers international cuisine at Willards Restaurant. For light snacks and cocktails, the hotel has Willards Bar, an ideal casual spot to meet with friends or colleagues.

The Hotel also provides complimentary access to the on-site Fitness Club. Additional services at the hotel include Free high-speed Internet access, Express Laundry with three-hour turnaround, Express Check-Out and Late Check-Out, Grab & Run Breakfast and Super Breakfast Buffet.

Accommodation has been reserved at the special rate of €179 for single occupancy (including taxes and breakfast). Further details for reserving accommodation will be sent to you when you register.

## Who Should Attend?

**Organic Chemists** – working in the pharmaceutical, agrochemical, flavours and fragrances, nutraceuticals and fine chemicals industries

**Development and Production Chemists**

**Chemical Engineers**

## Attendees will learn ...

Which equipment to use (exploratory screening, kinetic investigations etc.)

How to select the appropriate catalytic system (catalyst, solvent, acids,bases, modifiers)

How to properly determine the influence of pressure, temperature, mixing

What are the relevant experiments and how to interpret experimental results correctly

How to measure transport effects & how to determine the effect of transport limitations

What are the causes of catalyst deactivation and how to prevent deactivation

How to measure catalyst activity, selectivity and catalyst deactivation, changes in catalyst properties

How to determine the basic data (micro- and macro kinetics, thermodynamics, pathways) needed for a successful and direct scale up from laboratory to plant scale

How to integrate aspects of chemical reaction engineering

How to scale up successfully; scale up – scale down approach

When to run processes with suspended catalysts and when to use fixed bed reactors

Batch, semi-batch and continuous modes of operation

On the importance of back-and forward integration

How to estimate catalyst costs

How to handle catalysts safely and how to carry out catalytic processes safely

Many tips, rules of thumb, pitfalls

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