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FULL PAPER

«Catalysis: a unified approach»: a new course in catalysis science and technology

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Abstract
The need for enhanced education in catalysis is common to many countries. Dramatic progress in catalysis fundamental science and technology occurred in the last two decades enables teaching and learning of catalysis based on a unified approach in which catalysis including all its subdisciplines is taught in a logically consistent way using the organic chemistry reaction mechanism, namely the main chemistry conceptual methodology with its unique usefulness as predictive and creative tool. Selected lessons from the past are taken into account along with new insight on the role of catalysis and green chemistry in chemistry education based on systems thinking.

Keywords Education in catalysis · Career in catalysis · Green chemistry · Scientific skills · Catalysis subdisciplines

Introduction

Research in catalysis across the world is flourishing. The overall number of research articles in catalysis between 2006 and 2015 has grown at 5.78% annual growth rate (going from 6907 in 2006 to 11,303 publications in 2015) [1]. Not surprisingly, given the economic relevance of the scientific publishing industry [2], several new catalysis journals were launched by scientific publishers, including *ChemCatChem* (in 2008), *Catalysis Science & Technology* (2010), *ACS Catalysis* (in 2011), *Catalysts* (2011) and *Nature Catalysis* (in 2018).

However, whereas research in catalysis flourishes on a truly global scale [1], very few scholarly studies have addressed education in catalysis. In one of them, Murzin and Lokteva reported that during a 2015 international conference, a symposium on education in catalysis was held at the beginning of the conference regardless of the "European Federation of Catalysis Societies agreeing to arrange the symposium somewhat reluctantly" [3].

"To the surprise of the organizers" the symposium "attracted a lot of participants" [3]. Murzin and Lokteva found that very little information was available about education in catalysis in Europe even though it was clear that "in many European countries such as Finland as well as in the US there is no coordination between universities in terms of the number of courses devoted to catalysts, its content and structure" [3].

The need for such coordination emerged and was addressed in Germany in the early 1990s when, "it was felt that a dedicated curriculum for teaching catalysis was needed" [4]. The curriculum (*Lehrprofil Katalyse*) was created in 1993 and is continuously updated until today" [5].

Recent calls for enhanced education in catalysis are common to many countries. For instance, Dumeignil and coworkers in France in 2016 emphasized the need for establishing new courses throughout the world focusing on heterogeneous catalysis for the biorefinery encompassing many different fields in a multidisciplinary approach [6].

Issues with catalysis teaching, remarkably, were reported as early as of 1946 when Campbell wrote in *The Journal of Chemical Education* that 12 chemistry textbooks wrongly defined catalysts "as substances which alter the rate of a chemical reaction but are not themselves permanently changed" [7], when, Campbell continued, "a catalyst is a substance which affords a new mechanism for the reaction with no change in the chemical composition of the catalyst, though the catalyst actually undergoes permanent change" [7].

Accordingly, four decades later the International Union of Pure and Applied Chemistry will define a catalyst as "a

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substance that increases the rate of a reaction without modifying the overall standard Gibbs energy change in the reaction" [8] being "both a reactant and product of the reaction" [8].

Another issue in catalysis education is the separation between catalysis science and catalysis technology. I have lately discussed elsewhere the reasons for which, driven by global societal megatrends concerning the environment, health and energy, the chemical industry, which in the decades following the early 1980s became renown for its lack of process innovation, might shortly undertake both accelerated process and product innovation [9]. In this context of change, new catalysis science and technology such as heterogeneous catalysis under flow [10], single-atom catalysis [11], and heterogeneous catalysis applied to advanced biomaterials production [12], assume new practical relevance for the chemical industry at large (fine and specialty chemical and bulk chemical sectors).

Such accelerated innovation requires new collaboration between academic scholars and the chemical industry, including the catalysis industry which is an eminent part of it. Indeed, for instance, in Switzerland (home to a large and advanced chemical industrial sector) industry's and academic researchers lately started to increasingly reunite in meetings having "a much wider breadth than a typical catalysis course in an academic curriculum" [13].

New collaboration with industry includes that with flow chemistry companies many of which have routinely incorporated educational services aimed to customers until then completely unaware of the technology. As put it by Noël in 2019, indeed, "the chemistry curriculum still focuses almost exclusively on round-bottomed flasks - flow chemistry is not even mentioned." [14]

In this study I outline a new course in contemporary catalysis based on a unified approach in which catalysis including all its subdisciplines (homogeneous and heterogeneous catalysis, biocatalysis, electrocatalysis and photocatalysis) is taught in a logically consistent way using the organic chemistry reaction mechanism, namely the main chemistry conceptual methodology with its unique usefulness as predictive and creative tool [15]. Selected lessons from the past are taken into account along with new insight on the role of catalysis and green chemistry in chemistry education based on systems thinking.

Outline of the course and tools

Table 1 summarizes the subjects, learning outcomes and teaching methodology of «Catalysis: A unified approach» innovative course intended as a stand-alone graduate course.

Integrating teaching through contemporary research and using a historical approach [16], the course lasts two months (8 weeks, 4 h per day from Monday through Thursday). Lectures start presenting the historical development of catalysis [17], showing how the main subdisciplines of catalysis actually emerged from the split of chemistry into four main subdisciplines (inorganic chemistry, organic chemistry, physical chemistry and biochemistry).

The aim of the course is similar to that anticipated in 1999 by Notheisz and Smith with their course on heterogeneous catalysis in organic chemistry [18], namely to foster creativity through which today's students turned into tomorrow's researchers will solve open problems in making existing and unknown substances via new catalytic processes enabled by the invention of new catalysts and new conversions.

I have discussed elsewhere the substantial benefits of renewed chemistry education fostering creativity using contemporary research outcomes along with visualization and connectivity resources of the digital era [19].

Similarly, in agreement with the systems thinking approach to green chemistry education in the academy [20], teaching is delivered by instructors who include academic and industry's

Table 1 «Catalysis: A unified approach» - Outline of the course (Adapted from Ref. 11, with kind permission)

Subjects	Learning outcomes	Teaching methodology
The basics of catalysis and its historical development History and structure of the chemical industry and recent trends The scope and economic reasons of the transition from oil and fossil fuels to the bioeconomy Quantum chemistry, spectroscopy and microscopy in catalysis Homogeneous and biocatalysis Heterogeneous catalysis Single-atom catalysis Photocatalysis and electrocatalysis Catalysis in flow vs. catalysis in batch	After completing the course the students can: Demonstrate knowledge of the principles and key applications of catalysis Explain the relation and differences between catalysis various subdisciplines Explain the interdisciplinary connection of catalysis with materials and surface science Explain different catalyst preparation methods Explain use of quantum chemistry in catalysis, and modern catalyst characterization methods Identify and understand the latest knowledge connected to catalysis research	Teaching delivered in small classroom promoting active learning via a guided participation process Real time questions and answers, whole-class discussions Students challenged to present a research project in catalysis using simple, unifying and jargon-free terms Lectures from industry's researchers and managers Career forum: presentations and advice from industrial and academic researchers discussing career pathways Lectures, presentations and teaching materials on course website

researchers in a proper balance to promote understanding of the role of catalysis in the economy and society.

The aforementioned systems thinking approach [20], indeed, calls for the need to strengthen the interconnections between students and instructors on one side and society on the other (the interconnected elements of the system) including perspective employers (catalyst manufacturers and the chemical industry), and external stakeholders including environmental protection agencies and activists.

Teaching takes place in a small classroom (maximum 15 participants per course) promoting active participation via frequent thought-provoking questions so as to make the education personal. Since active learning is a guided participation process in which students engage in active doings (listening, speaking, reading, writing, and project execution) [21], students are guided by the instructor to develop new skills and new knowledge for each of the learning outcomes of the course (Table 1).

All presentations given at the course are video-recorded and the videos made available on the course intranet network for reflective practice of both students and instructors.

After completing the course the students will be able to: *i*) demonstrate knowledge of the principles and key applications of catalysis; *ii*) explain the relation and differences between catalysis various subdisciplines; *iii*) explain the interdisciplinary connection of catalysis with materials and surface science; *iv*) explain different catalyst preparation methods; *v*) explain use of quantum chemistry in catalysis and modern catalyst characterization methods; *vi*) identify and understand the latest knowledge connected to catalyst research.

Heterogeneous Catalysis: A case study of how flow chemistry is integral to a Catalysis class

As shown in Table 1, the course has many themes. To demonstrate how flow chemistry is important, I will examine the teaching of today's heterogeneous catalysis under flow as the key enabling technology of heterogeneous catalysis in the fine chemical and pharmaceutical industries.

Rather than using a conventional batch reactor in which the solid catalyst is stirred in the presence of the reactants, now the solid catalyst is placed in a flow reactor in the form of a packed powder or a thin coating, and the reaction mixture is flown through the reactor with reaction and separation of the catalyst from the reaction mixture taking place at the same time.

The instructor explains how the inherently safer and greener conditions due to the enhanced substrate:catalyst ratio combined with the enhanced mass transfer (much shorter diffusion paths), the efficient heat transfer, the low operating volumes and ease of scale-up (by parallel processing or process intensification) allow to dramatically lower production costs *and* enhance product quality in fine chemical and active pharmaceutical ingredient (API) manufacturing [21], a field dominated for more than a century by the batch reactor.

This, it is further explained, requires the development and the use of new generation heterogeneous catalysts of sufficient pore size (mesoporous) and large surface area in contact with the fluid dissolving the reactants thereby offering low flow resistance also due to the absence of swelling as it happens, for example, with organosilica-based sol-gel catalysts [22], or porous carbon nitride [23].

Seen from this new perspective, heterogeneous catalysis in flow is presented as a disruptive chemical technology capable to afford valued fine chemicals and ingredients of enhanced quality (purity), at a fraction of the cost and of the environmental impact of conventional industrial catalysis in batch [24].

For example, the oxidation of benzyl alcohol to benzaldehyde mediated by the solid catalyst Silia*Cat* TEMPO sol-gel entrapping the 2,2,6,6-tetramethylpiperidine-1-oxyl nitroxyl radical within an organosilica matrix with NaOCl as primary oxidant requires cooling at 0 °C and the use of KBr as co-catalyst to afford benzaldehyde in 97% yield after 1 h [22].

Under flow, using a simple tube reactor (T-piece, Fig. 1) adaptor enabling the flows of reagents to be combined at the input of the reactor charged with the solid phase, allows to reduce the reaction time down to 0.3 min, with 100% yield in

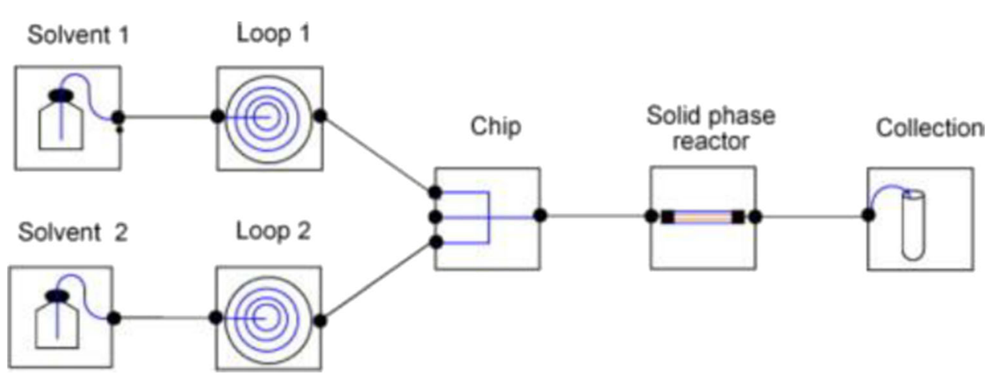

Fig. 1 Fluidic set-up for the heterogenous oxidation of benzyl alcohol in flow over Silia*Cat* TEMPO. [Reproduced from Ref. 22, with kind permission of Elsevier]

benzaldehyde at room temperature, with no need of KBr, a known corroding agent, as co-catalyst [22].

Alcohol selective oxidations mediated by TEMPO are ubiquitous in today's fine chemical and pharmaceutical industries [25]. After the homogeneous reaction, extensive purification of the API from residual nitroxyl radicals is required due to genotoxicity of TEMPO [26]. The continuous process over the Silia*Cat* solid catalyst not only allows to dramatically lower the reaction time eliminating the co-catalyst, but also eliminates the expensive product purification process.

Alone, this example show why the switch of the pharmaceutical and fine chemical industries is inevitable.

Still, as of late 2019 scholars in the US found that very few universities offer tailored courses on continuous flow chemistry [27], case studies and well designed experiments are used to demonstrate how, in practice, manufacturing fine chemicals and active incgredients using flow reactor technology consumes considerably less solvents and reactants allowing far better control of chemical reactions [28].

The key industrial requirements for commercial solid catalysts (high selective activity, long lifetime under real process conditions, and affordable cost) are presented, discussing the reasons for which academic studies for *decades* devoted little attention to the key issue of catalytic material decomposition and degradation [29].

Similarly, the instructor trains students on the importance of the catalyst shape for a commercially viable catalyst for processes under flow since, as put it be an industry's researcher at a recent catalysis workshop reuniting academic and industrial researchers, the catalyst shape often becomes the main driver of the performance of a catalyst in a commercial reactor [30].

It is not surprising, given the aforementioned ongoing lack of tailored courses on catalysis flow chemistry in most universities [27], that significant knowledge and skill gap are reported in the job marketplace, thereby creating room for intensive training courses on practical catalysis aimed at process, medicinal and production chemists wishing to "maximise their knowledge and understanding of catalysis being applied in organic synthesis and maintain their awareness of emerging catalytic chemical technologies" [31].

Students are therefore informed through a dedicated lecture on job opportunities and professional career how shaping advanced practical knowledge on heterogeneous catalysis under flow for synthetic organic chemistry provides them with unique advantages that will be crucially important for their careers in the fine chemical and and pharmaceutical industries.

Assessment, evaluation and reflective practice

Student assessment serving the purpose to show evidence that the course is effective in meeting its educational aims (Table 1) is done at the end of the course following again a systems thinking approach based on problem-based learning [32], by tasking each student to choose a real-world and challenging problem that in principle can be solved with new catalysis technology. Hence, the student is required to suggest suitable solutions to the problem identified based on today's catalysis science and technology.

One such authentic and relevant problem could be metal contamination of APIs used to manufacture drugs, namely the amount of residual metal used as catalyst in one of the reactions used to manufacture the API exceeding the maximum acceptable threshold [33]. How can heterogeneous catalys under flow be used to solve the problem? What are the technical and economic obstacles to be overcome? What is the role of workforce education in the uptake of catalysis under flow to solve this problem?

Following a formal presentation of the solutions suggested, feedback in written form is provided by the main instructor to inform the student of where and how their learning and performance can be improved in relation to the aforementioned broader learning outcomes. A final presentation incorporating changes suggested by the instructor is given by the student for final evaluation in front of a commission including one of the external educators.

Eventually, evidence for effectiveness of the course is assessed by collecting feedback from its users: namely students and employers. Hence, after the course information from trainees and their future employers is collected and used to inform reflective practice through which the educator studying his or her own teaching methods, determines what works best for the students [34].

After each course such reflective practice reveals evidence of successful aspects of the educational experience, so as to "amplifying what went well" [35], and the problematic aspects and the limitations of it so as to *specifically* act to overcome them and improve the future editions of the course [35].

Outlook and conclusions

This study describes a new stand-alone graduate course on catalysis based on a unified approach aimed to foster creativity [19] through which students turned into tomorrow's researchers will solve open problems in numerous fields impacted by catalytic phenomena through the invention of new catalysts and new catalytic conversions.

After summarizing the subjects, learning outcomes and teaching methodology inspired to the principles of systems thinking in green chemistry education [20], I use an example of how flow can be incorporated through discussions on heterogeneous catalysis. Numerous other examples of how flow chemistry that have an impact in the teaching of other forms of catalysis are possible and actually used in the course, starting from the emergence of photocatalysis under flow driven by visible-light to make fine chemicals and APIs [36, 37].

For example, students are shown how the invention of the flow photoreactor comprised of a transparent fluoropolymer tubing wrapped around the lamp [38], opened the route to the industrial utilization of photocatalysis (until then inherently limited by the poor light absorption of catalysts and reactants in solution typical of photochemical batch reactors) for the waste-free manufacture of fine chemicals, preferably and increasingly using visible-light (and not only UV radiation) as reactant [36, 37].

On leaving the course, after receiving advice from industrial and academic researchers discussing career pathways during a dedicated career forum part of the curriculum, students remain in contact with both the main instructor and the peers offering valued information used by the scholars organizing the course to inform reflective practice [35] by which the course is continuously improved, one edition after another.

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Compliance with ethical standards

Conflict of interest The author declares no conflict of interest.

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