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A Scientometric Analysis of Catalysis Research

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ABSTRACT

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The outcomes of the present scientometric analysis of research in catalysis provide chemistry and catalysis scholars with a closer bibliometric knowledge of an old and central field of chemical research which is being reshaped by fundamental and technological advances spanning from single-atom heterogeneous catalysis to flow chemistry. Improving and widening research and education in catalysis is a strategic need for national economies. Four research policy guidelines aimed at fostering progress in catalysis research and education conclude the study.

1. Introduction

Almost as old as chemistry as a modern science based on elemental composition of matter and chemical analysis principles formulated by Lavoisier in the late 1700s, catalysis entered chemistry research in 1835 when Berzelius introduced the term "catalysis" to indicate "the decomposition of bodies by this force in the same way that one calls by the name analysis the decomposition of bodies by chemical affinity".[1]

According to Berzelius the catalytic force in question, "very different from chemical affinity", was exerted by "simple and compound bodies" on other bodies.[1]

An instructive account on the historic development of the catalysis concept and its explanation was published by Wisniak in 2009.[2] The study goes from Berzelius until the first two Nobel prizes awarded in 1909 to Oswald and in 1912 to Sabatier, for his work improving the hydrogenation of organic species in the presence of metals, namely the catalytic hydrogenation of unsaturated organic molecules using "finely divided" Ni obtained by reducing nickel hydroxide with H_2 at 250 °C.

A brief but interesting history of catalysis dividing its historical development into five distinct periods was published by scholars in Sweden in 2013.[3]

Only a few scientometric study on catalysis have been published so far. In 2014, Zibareva and co-workers published two bibliometric analyses. Aimed to identify "hot topics" in catalysis research the first identified photocatalysis, electrocatalysis, stereoselective catalysis, biocatalysis, catalytic functionalization of organic compounds, nanocatalysis via graphene-based materials, biofuel catalytic production, and catalysis in new energy technology.[4] The second, based on a bibliometric analysis of publications including the term "nanocatalysis" concluded that "nanocatalysis" was a new research subject pertaining both to nanotechnology and to catalysis science.[5]

Though focused on a scientometric assessment of Indian publications in catalysis between 2006 and 2015, the first comprehensive study on catalysis was reported by Siddaiah and co-workers in 2016 in an open access journal aimed at librarians and at information scientists.[6]

The overall number of research articles in catalysis was found to have grown at 5.78% annual growth rate, going from 6,907 publications in 2006 to 11,303 in 2015.[6]

These findings are consistent with the rapid growth in knowledge production in chemistry between 1990 and 2009 due to profound changes in the chemical research process with a clear shift towards multidisciplinary and collaborative research carried out by scholars from other disciplines and from different countries.[7]

Catalysis is at the core of chemical manufacturing, not only of hydrocarbon fuels in various oil refineries around the globe but also of virtually all chemicals, including both bulk and fine chemicals. Virtually all catalytic technologies employed in industry are proprietary.

Once the patents have been filed, industrial researchers too seek publication in chemistry and catalysis journals since "publication becomes… a valuable tool to profile the expertise of a company to the scientific community and find partners, in order to initiate bilateral collaborations or other publicly funded projects with university. In a similar way, the innovation potential of a company becomes visible via publications, increasing its prestige".[8]

The paucity of scientometric studies in catalysis science and technology is accompanied by a similar low number of studies devoted to contemporary catalysis education, regardless of the widespread need perceived in many countries for better education in catalysis.[9,10]

This study critically presents the outcomes of a scientometric analysis of research in catalysis. Discussion is put in context of scientific publishing in the digital era, with preprints slowly but inexorably impacting the dissemination of chemical knowledge,[11] as well as of the renaissance of chemical manufacturing due to the concomitant emergence of new catalysis science and new process chemistry technology.

Chemistry researchers, including catalysis scholars, need a closer knowledge of scientometric tools like the h-index[12] and of scientometry in chemistry. Indeed, regardless of thoughtful pleas for quality and scientific impact evaluation of researchers based on examining the published papers only,[13] metrics-based such as the h-index are regularly used by universities and research agencies as a "decision-making tool" to evaluate both single researchers and entire university departments (via the mean h-index of the researchers working there).[14]

We agree with Barnes: the scholarly debate on science metrics currently confined to highly technical discussions in specialised journals[13] needs to shift from the latter journals to the main scientific journals and preprint servers regularly used by researchers active in that field. This study serves this scope in the important chemistry research field of catalysis.

The research policy guidelines concluding the study are aimed at fostering progress in catalysis research, education and industrial uptake in economically developed and developing countries.

2. Researching and publishing in catalysis

Ending his "On Catalysis" Nobel lecture given on December 12, 1909, Ostwald noted how the scientific field of catalysis was "in the first stages of its development. At present the main task is still essentially to discover and scientifically to establish the various cases of catalysis".[15]

Sabatier followed suit publishing in 1913 *La Catalyse en Chimie Organique*,[16] a book so rich of valued information about the fundamentals of catalysis that its 1922 translation in English is still read and commented at advanced catalysis courses more than a century later.[17]

The first catalytic use of gold, till then considered chemically unreactive, was reported in 1913 by Fokin who used asbestos as support of the finely divided gold nanoparticles in a industrially important reaction as the oxidation of methanol to formaldehyde[18] (today chiefly carried out in industry using a silver catalyst).

Fokin discovered also that Au and Ag powders were more active than supported Pt. Sabatier referred to Fokin's work in *La Catalyse en Chimie Organique*. Eventually, the latter book in 1922 was translated into English,[19] but these published findings were forgotten until Haruta and co-workers in 1987 reported the high catalytic activity of nanoparticulate gold in low-temperature CO oxidation.[20]

In general, since Sabatier's times the most important achievements of research in catalysis were published in general chemistry journals.

The first international catalysis journals specifically devoted to catalysis was *Kinetics and Catalysis*, namely the English translation of the Russian journal *Kinetica i Kataliz* founded in 1960 by Boreskov, Balandin and other prominent scientists at the Academy of Sciences of the USSR. Two years later the *Journal of Catalysis* was established by the Academic Press.

Table 1. Catalysis journals launched since the early 2000s

Journal	Year of launch	Publisher
Advanced Synthesis & Catalysis	2001	Wiley-VCH
ChemCatChem	2008	Wiley-VCH
Catalysis Science & Technology	2010	RSC Publishing
ACS Catalysis	2011	ACS Publishing
Catalysts	2011	MDPI
Modern Research in Catalysis	2012	SCIRP
Current Catalysis	2012	Bentham Science
Nature Catalysis	2018	SpringerNature

In the preface to the first issue of *Catalysis Reviews* launched in 1968 Heinemann wrote "catalysis is involved in one or the other step of manufacture of almost one-half of our industrial and agricultural product, yet it is less structured, less understood, still less of a science and more of an art than many other fields of smaller importance to our daily lives".[21]

Elsevier started to publish the *Journal of Molecular Catalysis* in 1975, followed in 1981 by *Applied Catalysis*. The latter journal was split in two sections in 1988, shortly after the 1987 launch by the same publisher of *Catalysis Today*. Only another publisher, Springer, had two journals in the field, *Catalysis Letters*, introduced in 1988, and *Topics in Catalysis* in 1994.

Reflecting the rapid rise of publications in the field occurred since the early 2000s,[6] several scientific publishers established new catalysis journals (Table 1). All these and related catalysis journals today publish research articles and reviews from all types of catalysis including heterogeneous catalysis, homogeneous catalysis, biocatalysis, electrocatalysis, photocatalysis, nanocatalysis, and organocatalysis.

Following the 1950-1977 development of organometallic catalysis,[22] for which in 1963 the Nobel prize in chemistry was awarded to Natta and Ziegler for olefin polymerization, and to in 1973 Fisher and Wilkinson for new olefin hydroformylation catalysts, the prestige of catalysis as academic discipline increased again since the early 2000s.

In 2001 Noyori and Knowles became Nobel laureates for their work on chirally catalysed hydrogenation reactions, and Sharpless for his work on chirally catalysed oxidation reactions. In 2005, Chauvin, Grubbs and Schrock were recognized for the development of the metathesis method in organic synthesis. In 2007, Ertl was awarded the Nobel prize for his studies of chemical processes on solid surfaces (including study of the nitrogen fixation mechanism in the Haber –Bosch process for ammonia synthesis), followed in 2010 by Heck, Negishi, and Suzuki for cross-coupling catalytic reactions and by Arnold in 2018 for the directed evolution of enzymes.

Similarly to what happened with the chiral ferrocenylphosphine ligands for asymmetric catalytic hydrosilylation of ketones introduced in 1974,[23] the new catalysts introduced by the aforementioned scholars and by several other chemists today are widely used for manufacturing fine and specialty chemicals, vitamines and other active pharmaceutical ingredients.

The almost contemporary emergence, in the early 1990s, of nanochemistry and green chemistry oriented to waste-prevention rather than waste control, drove a second wave of progress in catalysis science and technology.

A number of newly developed bottom-up material synthetic routes, such as sol-gel and hydrothermal often “assisted” by microemulsion templates, along with new surface chemical functionalization strategies enabled the replicable preparation of nanostructured catalytic materials of high selective activity easily recovered and reused;[24] suitable for use for example in producing pharmaceutical “generics” with dramatically reduced reaction times, solvent utilization and waste production.[25]

Conventional production routes used in manufacturing fine chemicals (10,000 t/a demand) and pharmaceuticals (1,000 t/a demand) prior to the introduction of green chemistry production processes typically generated 100 kg and 50 g of waste per kg of manufactured product.[26]

3. Scientometric analysis

The scientometric assessment of research in catalysis referring to the 2006-2015 period shows that China led the ranking with 28.12% of the global share of research articles in the field, followed by the USA with 14.93% of the share.[5] The other countries in the ranking were Japan, India, Germany, France, South Korea, Iran, Spain and Great Britain. Together these first 10 countries account for 82.45% of the global publication share in the catalysis research output.

Table 1. Top 10 most productive countries in catalysis research 2015- 2020 (June 11th) (Source: Scopus, 2020)

Ranking	Country	Number of papers	Share of papers (%)
1	China	18,533	38.4
2	USA	7,824	16.2
3	India	3,800	7.9
4	Germany	3,285	6.8
5	Japan	2,798	5.8
6	Great Britain	2,052	4.2
7	Spain	1,876	3.9
8	France	1,809	3.7
9	South Korea	1,588	3.3
10	Iran	1,451	3.0

Following the same approach a scientometric assessment of research articles in catalysis published in indexed scientific journals between 2015 and June 11, 2020 (Table 1) was readily obtained by carrying out a search on Scopus using the words “catalysis” or “catalyst” present in the title, abstract or keywords.

Limited to documents published in English in the form of research articles or reviews (excluding book chapters, conference papers and *erratum* communications), the search returned 48,257 documents. Of these, 48,169 were published in scientific journals, 81 in book series, and 7 in trade journals.

Interestingly the share of the leading countries even increased in the last five years amounting to 93.2% of all papers in English published in journals indexed by Scopus, with China (38.4%) dominating even further. Germany surpassed Japan, and Iran managed to remain amid the world’s top 10 countries for research in catalysis regardless economic sanctions that, for example, slow down or even impede purchase of chemical reactants from academic laboratories in that country.

Other countries worth mentioning are Italy (11th in the global ranking, with 1,226 papers) and Russia (12th in the rank, with 1,111 papers). Russia, for example, hosts since 1958 the world largest academic centre in the field Boreskov Institute of Catalysis, part of the Russian Academy of Sciences.[27]

In Russia, since the 2006 new science policy allocates funds and grants depending on the research assessment based on publications in the international literature. The number of research papers published in English all scientific fields including chemistry dramatically increased. The current policy in Russia also drives institutions outside of three main scientific cities (Moscow, St. Petersburg and Novosibirsk) to enter the international arena in a way similar to that followed by China in the last three decades with several leading universities and research centres today located well beyond China’s two main cities (Beijing and Shangai).

Table 2. First 10 institutions in catalysis research 2015- 2020 (June 11th) (Source: Scopus, 2020)

Ranking	Country	Institution	Number of papers
1	China	Chinese Academy of Sciences	3,299
2	China	Ministry of Education China	2,785
3	China	University of Chinese Academy of Sciences	1,210
4	France	Centre National de la Recherche Scientifique	996
5	China	University of Science and Technology of China	709
6	China	Tsinghua University	620
7	China	Zhejiang University	528
8	China	Dalian Institute of Chemical Physics Chinese Academy of Sciences	496
9	China	East China University of Science and Technology	460
10	China	Tianjin University	460

Indeed, amid the first ten institutions only one (France’s CNRS) is not Chinese (Table 2). Across the world it is governments, and not chemical companies, to provide funding to catalysis scholars (Table 3).

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Table 3. Top 10 organizations funding catalysis research 2015-2020 (June 11th) (Source: Scopus, 2020)

Rank	Funder	Number of papers
1	National Natural Science Foundation of China	12,265
2	National Science Foundation (USA)	2,147
3	Fundamental Research Funds for the Central Universities (China)	1,904
4	National Basic Research Program of China (973 Program)	1,398
5	Department of Energy (USA)	1,332
6	Japan Society for the Promotion of Science	1,021
7	National Institutes of Health (USA)	1,013
8	Chinese Academy of Sciences	953
9	Office of Science (USA)	886
10	Deutsche Forschungsgemeinschaft	885

It is also noticeable amid the top 10 journals chosen by the latter, only two journals specialize in catalysis science and technology (Table 4). One is an organic chemistry journal, one is devoted to communications in all fields of science, and the remaining 6 are multidisciplinary chemistry journals.

Table 4. Top 10 journals publishing catalysis research 2015-2020 (June 11th) (Source: Scopus, 2020)

Rank	Journal	Number of papers
1	Journal of the American Chemical Society	1,797
2	ACS Catalysis	1,734
3	Angewandte Chemie International Edition	1,546
4	Journal of Organic Chemistry	1,339
5	Chemical Communications	1,330
6	Chemistry A European Journal	1,049
7	ChemCatChem	1,035
8	ChemSusChem	745
9	RSC Advances	735
10	Nature Communications	720

Pointing to slow but increasing acceptance of the open access (OA) publishing model also amid chemists, out of 48,257 articles, scholars opted for OA publication in the case of 7,443 studies, namely 15,4% of the cumulative number of papers published.

The graph in Figure 1 shows that the yearly number of studies decreased to 7,708 in 2016 from 7,867 in 2015. But since then it has continued to grow at fast pace to reach 10.048 studies published in 2019.

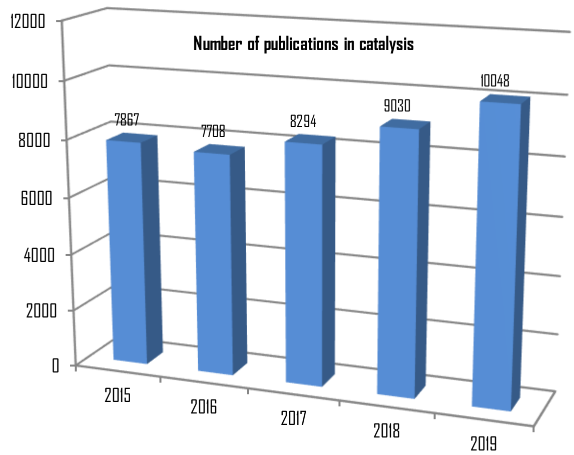

Figure 1. Yearly number of publications in catalysis science and technology, 2015-2019. [Source: Scopus, 2020].

To understand the scope of the growth of research in catalysis science and technology it is enough to learn that a similar search for research and review articles published in English limited to year 2000 returned 3,017 documents. In other words, the scientific output in catalysis has more than tripled, largely thanks to the ingress of new scholars based in Asia, chiefly in China and India, but also in South Korea and in Iran. An old research field historically dominated by scholars based in USA, Europe, Japan is now largely dominated by China. With over 1.35 billion inhabitants growing at fast pace, and a vibrant chemistry school growing rapidly in terms of quality, quantity, funding and international collaborations,[28] India's contributions to catalysis progress are poised to surpass contributions from the USA within the next decade.

4. Outlook and Conclusions

From the economic viewpoint research in catalysis is particularly important because, through further organic process development, it enables the production of virtually all chemical substances, including valued fine and specialty chemicals and active pharmaceutical ingredients (APIs).

Certainly utilization of continuous production technologies is a common place in production of fuels and bulk chemicals, However, utilization of the same practices in manufacturing of fine chemicals is reshaping the industry at the the global level. Until the advent of flow chemistry production processes, manufacturing fine chemicals and APIs, requiring significant capital and operational expenses (CAPEX and OPEX, respectively), was limited to European countries including those formerly part of the Soviet block and North America countries, and subsequently to China and India where productions were outsourced to companies identified in the chemical business jargon as "custom manufacturing organizations" (CMOs).[29]

Coupled to new generation heterogeneous catalysts, flow chemistry dramatically lowers both CAPEX and OPEX costs. The former costs are dramatically reduced because large batch reactors equipped with complex temperature, mixing and pressure control tools are replaced by one or more small flow reactors enabling far better controlled, safer and milder reaction conditions.

The latter costs fall because as already noted by Pollak in 2011 in the preface to his reference book devoted to the fine chemical industry the "most progressive companies adopt lean production principles originally developed for the automotive industry".[29]

Continuous production in small and modular flow reactors with new generation solid catalysts prevents the formation of unwanted by-products, eliminates the need for catalyst and product separation and shortens time to market. Production becomes truly driven by a demand preventing overproduction by recreating in fine chemical plants the same lean production mode used by the most advanced manufacturing industries.[30] The shift in the paradigm requires new skills and much broader utilization of chemical engineering practices, which were often in the periphery of process development focusing mainly on chemistry.

The increasing shortage of APIs, especially of generics, in many developed and developing countries culminated with shortage of hydroxychloroquine (HCQ) used to treat COVID-19 patients. Such situation , which in early 2020 led India to dramatically scale up production for donating the drug to more than 50 countries,[31] has made clear that countries cannot rely any longer on API and fine chemical imports.

The creation from scratch of a national fine chemical and pharmaceutical industry in African, Asian, Latin American and European countries is now possible. Followed by South Africa with 260 publications in the field of catalysis in the aforementioned 2015-2020 (early June) period, with 348 publications Egypt leads the rank of African countries. Algeria (117), Tunisia (111) and Morocco (91) rank third, fourth and fifth. The impact of COVID-19 epidemics in North African countries was very limited. In Morocco the government acquired all HCQ-containing drugs locally manufactured by a foreign company on March 2020.[32] Algeria took similar initiative at the same time negotiating with two pharmaceutical groups the purchase of large quantities of drugs using hydroxychloroquine as API both produced in Algeria and imported.[33] Tunisia begun manufacturing hydroxychloroquine locally.[34]

The latter non-steroidal drug with anti-inflammatory activity, a generic widely used also for the treatment of rheumatoid arthritis, can be manufactured under flow conditions with an yield improvement of 52% compared to the commercial process combining two packed bed reactors with one batch reactor used for heterogeneously catalyzed reductive amination and hydrogenation steps, affording direct conversion of the starting materials to HCQ.[35]

The example can be generalized. Most synthetic routes for the production of fine chemicals and APIs can now be carried out under flow using heterogeneous catalysts – including single-atom catalysts,[36] now approaching commercialization -- at a fraction of the cost of conventional routes in much smaller chemical factories scattered across countries. Under these conditions, the availability of chemistry professionals specializing in catalysis and contemporary process chemistry is an urgent need for all world's countries willing to become at least partly self-sufficient in the production of life-saving drugs as well as of a host of valued substances which are essential to virtually all sectors of modern economies.

In this context, improving and widening research and education in catalysis becomes a strategic need for governments and national economies. Four main guidelines, two for governments and two aimed at chemical companies, emerge from the present scientometric analysis and related studies on the global reshaping of the chemical industry.[37]

First, aware that catalysis and process chemistry are the key enabler technologies of the chemical industry, governments should support the creation of dedicated research centres as done for example in Russia with the Boreskov Institute of catalysis,[27] thereby letting the higher research and education institution to achieve the required sufficient dimension to act as purposeful partners of the chemical industry.

Second, aware that in most countries education in catalysis at the undergraduate level is generally not adequate, lacking uniformity[9] and suffering from obsolescence in a still fragmented approach to its sub-disciplines,[10] governments should follow the example of Germany, where such a national curriculum (*Lehrprofil Katalyse*) was created in 1993 and since then is constantly updated, asking universities to adopt a national curriculum.

Third, aware of the unique economic relevance of catalysis, chemical companies should start effective collaboration with public research centres thereby increasing the research and development (R&D) capacity of local firms and entrepreneurship and innovation capacity of young researchers. There are many ways to do that. Among examples known to the authors Germany, France, Finland and Switzerland should be mentioned. Worth emulating is Switzerland where regular professional workshops between industry's and academic researchers are organized.[38]

Fourth, chemical companies should learn from what happened to manufacturers of gas-powered turbines whose market shrank from 60 GW in 2014 to 31 GW in 2018,[39] due to completely unforeseen and rapid global uptake of wind and photovoltaic generation across the world.[40] Now that renewable power coupled with demand management with Li-ion batteries is cheaper than gas generation even without subsidies,[41] the market for gas-powered turbines will never recover.

The same will shortly happen with flow chemistry and new catalysis technology in chemical manufacturing. After more than two decades in which green chemistry remained mostly confined to academic research papers and conferences,[42] the falling cost of flow chemistry reactors coupled to the increasing availability of completely new heterogeneous catalysts provides an highly profitable business opportunity for all new fine chemical manufacturers. For example, using new gree technology new or existing companies might start producing the APIs of generic medicines in increasing shortage[43] at a fraction of the cost of competitors using old production technology in batch reactors.

Now that regulatory agencies in most countries allow the use of flow chemistry for manufacturing APIs and fine chemicals, it is enough to analyze the sales of industrial flow reactors to learn that the process has already started.[44]

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Notes

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