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Grand challenges in industrial catalysis: let's put academia and industry on the same page!

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Grand challenges for industrial catalysis

In its broadest sense, catalysis is playing an increasingly important role in the chemical industry due to its inherent advantages that combine high selectivity, efficiency, and often mild reaction conditions. Catalysis (traditionally classified as homogeneous, heterogeneous, and biocatalysis) is applied nowadays in the production of a wide range of (bio)fuels—of several generations –, bulk commodities, polymers, different (bio)plastics, or a broad array of optically active building blocks employed for pharmaceuticals and fine chemicals. The industrial implementation of catalytic processes is here to stay, also fuelled by the fact that catalysis is, in itself, one of the Green Chemistry Principles (number 9), what may contribute to the set-up of more sustainable synthetic procedures. Adding to that, synergies may be created by using (bio)catalysis in the on-going replacement of petroleum-based resources by a more circular paradigm—using biogenic raw materials –, what will broaden the use of greener concepts under industrial premises in the future (Domínguez de María, 2016).

When it comes to “Industrial Catalysis”, an important challenge to be highlighted is the difficulty to precisely define the real state-of-the-art of the different (bio)catalytic concepts investigated and/or implemented by industries. Thus, while the academic research follows the classical paths of publishing and dissemination activities—in the form of scientific publications, and conference presentations –, many industrial initiatives related to catalysis remain unpublished or are only briefly covered in the patent literature—which results often much less descriptive than academic papers. As a consequence, many relevant industrial catalytic processes—and the fundamentals and motivation of the research realized in industry –, may remain undisclosed, hindering their further development by research groups, or, worse, making academic researchers to *reinvent the wheel* in some cases, when non-disclosed topics are (re) investigated again. In this context, providing a solid dissemination framework where both industrial and academic researchers may feel comfortable to discuss their challenges and processes and contribute to the advancement of the field, would be highly beneficial for the broader implementation of sustainable catalysis at practical level. In fact, having access to a *virtually complete* state-of-the-art of industrial processes would stimulate the research in catalysis for academic groups too. Some publishing initiatives in that respect already exist, and it is important that more actions can be taken in that direction.

As stated above, catalysis is already—and will become even more in the future –, one of the pillars from which sustainable chemistry will be built. On that basis, it would be important to speculate what would be the main research lines that should be developed to reach a deeper penetration of catalytic technologies in industrial environments. Herein, such research needs for implementing industrial catalysis can be possibly contextualized (in an ample manner), through the triad “solvent-water-catalyst”, and ways to interconnect them to perform sustainable and efficient (bio)catalytic processes. In fact, the interphases

between solvents and water, and interactions with the catalysts will reveal to be crucial to understand and to build robust sustainable catalytic systems.

With respect to solvents, starting from mere mass-metric perspectives, e.g., how much solvent is used? or how much solvent can be recycled? etc., the discussion can necessarily be extended to the design of (bio)catalysts that can operate efficiently under *real* industrial conditions, and at interphase between solvents, water, solid resources, etc. In this context, the development of “media-agnostic” (bio)catalysts that can operate within a broad range of solvents and crude industrial effluents appears as highly important for future industrial catalysis (Milic et al., 2022). Related to the type of solvent to be used, although the implementation of solvent-free catalytic processes would always be the preferred approach—“the best solvent is no solvent”, whenever this may be possible –, the use of solvents for both the synthetic reaction (upstream) as well as for the product purification (downstream) is commonly observed in industrial processes. As solvent are used in large volumes, it is easy to do the math to assess their huge contribution to the environmental footprint of chemical processes (Hagen, 2015; Sheldon, 2023). Therefore, the identification of *greener* or at least more sustainable solvents for industrial catalytic performances appears mandatory (and challenging!) to reduce the environmental burden that synthetic processes may have (Jessop, 2011; Clarke et al., 2018). In that sense, the design of (bio)catalysts displaying high efficiency and selectivity in these media are a cutting-edge aspect for industrial catalysis; providing real (bio)catalysts for real practical conditions. Notably, the implementation of newly designed solvents must always be accompanied with the provision of an adequate quantitative assessment, reporting the environmental metrics that can clearly substantiate the improvements in the greenness of the process (Lange, 2021; Tulus et al., 2021).

Apart from solvents, chemical industrial processes are oftentimes highly water demanding. In fact, water finds uses in industry as solvent—as the prototype of the non-hazardous, readily available solvent –, as heating-cooling agent, or as washing agent during several downstream processing units, to cite some relevant examples (Cortes-Clerget et al., 2021). The use of water as solvent media for synthetic reactions has traditionally been implemented in biotechnology (Domínguez de María et al., 2023), and has gained interest in the last years for many chemical processes, combining chemo-enzymatic strategies (Lipshutz, 2023). Likewise, chemical plants need volumes of water to operate (e.g., steam-based systems), or to purify/clean products and devices after the synthetic procedure. Overall, as water is used in large amounts, its smarter use represents another stimulating and needed branch for research in Industrial Catalysis. Building up strategies in which (bio)catalysis can be combined with water effluents, and how water can be recycled, appear fundamental to reach sustainability. Furthermore, the way in which water is (re)used and ultimately treated as residue—by divesting it to Wastewater Treatment Plants (WWTP) –, is and will be of utmost importance in the future. Research in the direction of wastewater treatment of industrial (catalytic) processes will represent another stimulating field in which alternatives can be envisaged, e.g., use of catalysis as tool to remove recalcitrant chemicals in a sustainable manner (Krell et al., 2021; Domínguez de María et al., 2023).

Finally, an adequate (bio)catalyst design to cope with actual industrial reaction conditions while being efficient and selective is of

utmost importance. Herein, academic design results crucial to understand the performance, and propose ways to improve the catalytic efficiency, robustness, possibility of immobilizing and reuse it, etc. Likewise, process design and reactor set-up (e.g., assessing batch or continuous systems) are crucial areas to be explored thoroughly. And connected to that, the early assessment of catalysis under real industrial conditions (e.g., an impure solvent fraction, or presence of water, etc.), should not be overlooked, to assure that processes can be implemented and coordinated with further or previous synthetic steps in chemical pipelines. Once again, the cooperation between academic and industrial research appears necessary to reach these premises.

Overall, the cooperation between Academia and Industry will be key to success for future catalytic performances at practical scale. Industrial contributions showcasing real challenges, and ways to circumvent them will be highly helpful to define new academic questions to be addressed, for knowledge generation. Likewise, challenges encountered during scaling-up will be illustrative on what aspects need to be defined in a (bio)catalyst to its further practical implementation. Herein, Industry must take the lead in shedding light on real problems and needs, where Academia can then put capacity and talent to put forth innovative solutions. And on top of all of this, in this XXI century showing efficiency and selectivity in (bio)catalytic systems is not sufficient. There is also the need of quantitatively probing that sustainability is reached (or at least improved) in each new (bio)catalytic step that may be proposed for industrial applications.

Author contributions

PD: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Validation, Visualization, Writing—original draft, Writing—review and editing.

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