Catalysis Today 272 (2016) 2–5

Contents lists available at ScienceDirect

Catalysis Today

journal homepage: www.elsevier.com/locate/cattod

50 years in catalysis. Lessons learned

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A R T I C L E I N F O

Article history:
Received 7 June 2015
Received in revised form 10 August 2015
Accepted 12 August 2015
Available online 8 September 2015

Keywords:
Research management
Syngas
In situ methods
Scale-up

A B S T R A C T

Management of responsive research is a difficult balance between order and chaos. It is essential that each scientist has a room for initiative. Public research policy should focus on frontier research and not force universities into “non applicable applied research”. Long-term basic research is important for a high tech company to establish a two-way collaboration with academia and to ensure future options for the company. The challenges to industrial catalysis are discussed in terms of a SWOT analysis.

1. Introduction

My professional life has dealt mainly with catalysis [1] and research management and policy [2]. Most of the time I have worked with Haldor Topsøe. The research dealt mainly with syngas [1,3,4]. Another activity was working as a founding member for the European Research Council. This paper describes main impressions on how to promote responsive research and outlines the main challenges for the science of industrial catalysis.

2. The R&D game

2.1. The Topsøe experience

Haldor Topsøe applied a multiple approach to industrial catalysis [5]. He initiated research projects in parallel to the development work to understand the science behind the work. This gives the strength to cope with problems and is of course also of value for marketing. Part of this research can be published. It motivates scientists and it forms a basis for collaboration with university groups. It is important that this collaboration is a two way process to the benefit of both parties. It requires that the company is active in basic research as well [6].

Another attitude was the aim of being in front with core competencies around industrial catalysis ranging from computer methods to advanced methods for catalyst characterization and in situ studies [7]. Further development of core competencies yields competitive advantage and it creates the ability to catch opportunities and to ensure options for the future.

Finally, the multiple approach includes explorative research aiming at “radical innovation”, solutions for the next generation of technologies (the “second S-curve” [8,9]). In some situations this activity may be reduced to testing attempts in the scientific world or by competitors by “active monitoring” [5,9].

Haldor Topsøe played a decisive role in guiding and inspiring the scientists and by encouraging a cooperative approach. The work was organized in ad hoc, cross disciplinary project groups supported by a lean departmental structure.

It is of course a challenge to manage these parallel activities, in other words to find the balance between order and chaos. Management of innovative research is like growing a garden [5,10]. If everything is under control as in a baroque garden, it may look nice, but there are no surprises. If nothing is under control, there may be an interesting jungle with a lot of activity, but nothing new is likely to happen. The truth is in between. The art is to manage with a loose line, to make sure that each scientist has a room for initiative. One solution is to apply the so-called 65/25/10 approach [5] in which the numbers are only indicative. It means that 65% of resources within a project is used for the development work with well defined milestones and budgets. 25% is used by the team for its own solutions to the problem and 10% to any activity (skunk work) within the scope of the company. Before scaling up the activity a simple analysis should be made of the novelty of the idea and benefit to the client, the resources to establish the first sale, and the feasibility of the project for the company. The stage gate model may be used for large projects but it is a killer for projects in the explorative phase. Research should be managed by motivation, not by control.

The entire process of bringing “science to dollars” [6] is complex. It is important not to work with a linear process having basic

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http://dx.doi.org/10.1016/j.cattod.2015.08.033
0920-5861/

research or applied research and development following each other with the R&D making the results available before starting engineering and marketing. It is essential to work in a concurrent fashion and to manage the linkages between overlapping phases [5]. Typically, “strategic marketing” should start when there is a “proof of concept”. On the other hand fundamental research may continue long after these activities to understand better the key problems and to prepare for new solutions.

The key challenge for responsive research is to establish a balance between “focus and hokus pokus”, to avoid making the innovation process too bureaucratic and making sure that each scientist has a room for initiative.

2.2. The ERC experience

The European Research Council (ERC) was founded 2007 to promote and sponsor frontier research under the European Community’s Framework Program. It has been successful in giving grants to individual scientists with investigator-driven projects (bottom-up projects). Scientific excellence is the only criteria. However, excellence is a misused word. Scientific excellence is not much worth if it is not coupled to ambition, courage and passion. One trap is “fashionable research” being a result of the increased pressure to publish. Scientists then focus on “safe science” in areas with high citation rates and with little renewal.

Scientific excellence is sometimes considered higher if the activity has no relevance. However, a big part of fundamental research that is driven by curiosity and ambition only often leads to big break-throughs decades later. Meanwhile, another part of fundamental research may be directed to solve a specific problem. One example is Pasteur as described by “Pasteur’s quadrant” [2,11]. Hence excellence and relevance need not be in conflict.

Funding agencies and industry should of course focus on subjects and competencies considered relevant, but it is important to ensure a balance between research with “short term” relevance and research driven by curiosity and ambition. More and more often, discoveries are made in basic research which can rapidly be transferred into industrial developments and thus “short-circuiting” the conventional linear model for the R&D process [2,12]. This has also been demonstrated by the “proof of concept” scheme [13] giving start-up grants to ERC grantees seeing industrial or societal relevance of their projects.

Research policy is often guided by the so called linear model assuming a direct correlation between resources used locally and local growth. This is misleading as technology and science develop in parallel on the global scene [14]. The linear model assuming that university research leads to industrial innovation has caused an increased pressure on universities to do applied research in areas deemed to be relevant. However, with no feed-back from the market place this easily results in “non applicable applied research” [2]. The best transfer of knowledge form universities to industry is through candidates who have been trained in an environment of research at the borderline of our knowledge.

In conclusion, there are good reasons to sponsor fundamental research whether relevant or not and not be directed of the political pace of being relevant [14]. For the science of catalysis it means that there is a strong incentive to promote collaboration between fundamental research at universities and industry.

3. Challenges to industrial catalysis

3.1. A multidisciplinary effort

Industrial catalysis has been instrumental in the growth of the petrochemical industry, the fertilizer industry and the refinery industry. It is a multidisciplinary activity and it involves input from reaction kinetics, surface science, reactor modeling, and the technologies involved in the manufacture of catalysts [15]. It is the integration of these and several related competencies which form the field of industrial catalysis. Industrial catalysis is not just the behavior of the active site. It is coupled to complex interaction with mass and heat transfer. Moreover, it is rather the exception that the catalyst activity turns out to be the decisive factor in reactor design. Very often selectivity and secondary phenomena such as catalyst deactivation are more important [9].

3.2. Strengths

50 years ago the science of catalysis was based mainly on reaction engineering principles and vague ideas on the mechanism of the reaction. For metal catalysis the discussion was whether to explain catalytic phenomena on basis of bulk (collective) properties of the catalysts or in terms of “the individual surface atom”, “spill over” effects, etc. [1].

Today the science of catalysis has very strong tools available allowing a precise description of the catalytic reaction at atomic scale. Surface science resulted in a number of advanced characterization techniques. The main progress was made with the introduction of in situ methods [16].

A number of these contributed to the understanding of practical problems for a number of reactions studied by Topsøe such as studies in situ high resolution transmission electron microscopy (HTREM) of carbon formation on reforming catalysts [17], sintering of nickel catalysts [18], and changes of crystal shapes in copper catalysts for methanol synthesis and low temperature shift reaction [19]. In situ combined EXAFS/XRD was developed and applied for the study of several phenomena, as for example the activation of copper catalysts [20]. Scanning tunneling microscopy (STEM) developed by the Besenbacher group at Århus University was used for identification of the active BRIM site in hydrotreating catalysts [21]. The experimental work was supported by the development of Density Function Theory (DFT) calculations by the Nørskov group at Denmark’s Technical University. It was possible to predict the optimum catalyst for the ammonia synthesis [22] and by using the “scaling principle” [23] to predict catalyst activity for the reforming reaction [24] and to explain the mechanism of carbon formation [25]. A fruitful collaboration emerged between the Topsøe research group and these two university groups almost forming a Danish school of catalysis. The joint activity was based on openness with the ambition of being leading in the selected field.

In parallel with the development of surface science the computer methods [9] lead to more sophisticated models for simulation of the catalytic reaction at industrial reactor conditions. These were able to consider mass and heat transport to the catalyst pellets as well as axial and radial temperature and concentration profiles through the reactor bed. Non ideal flow was handled by CFD (computational fluid dynamics).

The strengths in fundamental work and in reactor modeling formed the basis for a more efficient method for scale up of catalytic processes [9,26]. Instead of the traditional bench scale testing giving limited information for design an early scale up was made to pilot scale at industrial mass velocity and heat transfer rate. At this scale results are relevant for engineering of industrial units and the constants in the reactor models can be determined thus providing a strong tool for design of industrial plants.

Practice has also shown that it is at this scale that secondary phenomena such as unforeseen deactivation are best recognized. The fundamental knowledge from surface science can be applied when studying the spent catalyst samples from the pilot testing. This is done by the advanced characterization methods and by dedicated scale down experiments. The results give feed back to the