Catalysis Today 178 (2011) 8–11

Contents lists available at ScienceDirect

Catalysis Today

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

So you think you may have a better process: How can you define the value?

John N. Armor*

GlobalCatalysis.com L.L.C., 1608 Barkwood Dr., Orefield, PA 18069 USA

ARTICLE INFO

Article history:
Received 5 May 2011
Received in revised form 28 May 2011
Accepted 30 May 2011
Available online 30 June 2011

Keywords:
Applied catalysis
Value
Markets
Marketing
Industrial catalysis
Chemical and petrochemical processes

ABSTRACT

This perspectives article is intended to help scientists, particularly in catalysis, understand how to assess the value and impact of research with potential, practical value. These remarks are also offered to help scientists develop added value for new discoveries in catalysis. Authors are encouraged to seek input about process or product improvements before making sweeping statements about the impact or implications of the work. At the same time, the intent is not to contrast fundamental or applied catalysis, but to provide the reader with a perspective and resources for assigning value to their work. Specific suggestions are offered on how to begin to gather such expert information and use that to build or guide one's further research. Topics include gathering cost information, looking at the total process, including energy assessments, life cycle assessments, and sensitivity analyses. Brief examples using the H_2, NH_3, and CO_2 markets are given.

1. Scope of assessment

So often one reads of far-reaching claims from or attributed to scientists about a discovery regarding the performance of a new catalyst, but without any reference to the process hurdles, the market, or comparisons to existing technology. This manuscript seeks to help the reader understand the importance of getting some assessment of real value, understanding hurdles towards eventual application, and gathering market information early in one's research. When pursuing research towards an intended application, understanding the limits of existing technology is certainly an important aspect in undertaking any new research project, but unless one understands where the catalyst of focus fits with regard to existing technology or what are the limitations of the existing technology, new research could end up going in an ineffective direction. I am not talking just about the sales price or material yield, but about processing conditions, reaction parameters, equipment and capital costs, operating costs, etc. Understanding what the market is and also the demands of the customer are crucial in providing a successful replacement or alternative technology. What I will try and do is to show readers that if they want to claim their work is valuable for reasons of a particular product or displacing an existing process, than they need to first gather information about the market and the entire process for producing that product in order to benchmark their discovery.

When I use the term "market," it is not in the traditional business school sense of sales, advertising, and distribution, but really about the demand by the marketplace for a product. If one wants to sell a product in a free marketplace, it has to be competitively priced (where it is not being influenced by tariffs or government) to meet demand by customers, which usually means that it needs to be produced more cheaply and efficiently than alternative products of similar value or composition in the current marketplace. Having a full understanding of what sets the price of a material is crucial to understanding the value of new versus existing products. Such understanding often builds with time on a project and searching the marketplace.

2. Units of cost and estimating potential price

A good place to start with assessing any alternative technology is the cost and availability of the feedstocks. The chemicals and petrochemical business often cite the cost of chemicals on per unit volume, mass, or unfortunately some other non-uniform unit. Obviously, in making comparisons between feedstocks and relating them to products one must use the same basis of units. Begin by just summing the costs of all reactants against the cost of all products. When co-products are produced, it is usually not fair to assume they would all sell at existing market prices. Co-products often have lower value versus their market price. For example, we know [1] that on a mass or mole basis a lot more ammonium sulfate is produced during the production of caprolactam using the popular phenol based route, but so much by-product ammonium sulfate has limited value depending on other factors, such as where

* Tel.: +1 610 3951406.
E-mail address: GlobalCatalysis@verizon.net

0920-5861/$ – see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.cattod.2011.05.036

it is produced (Does it have to be shipped to a customer?), is it a seasonal product, would one be saturating a local market, does it require a challenging level of purification for another customer, etc?

3. Looking at the total process

Intuitively, reducing the number of process steps or unit operations, the temperature, the pressure, improving selectivity [2], or the use of cheaper metals in the catalyst would be expected to reduce the cost of the product, but one has to complete that thought and ask, by how much? Many processes are controlled by factors that may make a new catalyst or a change in reaction conditions unattractive. The cost to change equipment, the cost to develop a new, commercial grade catalyst, the regional feedstock costs, the cost of any new investment, as well as many non-obvious factors can significantly impact the price of a product and thus reduce the perceived value of a new discovery.

Just looking at one step of a multi-step process is not a fair way to compare prices of one product versus another. One has to look at all the steps of all alternative processes and consider the added processing costs of operations like compression, distillation, purification, separation, etc. that might be required to get to the desired product. Any of these processing steps, not apparent in the net reaction of a process, can often negatively impact the acceptability of a process moving to the commercial scale. One has to understand what determines the price of the material in the marketplace. The chemicals marketplace is certainly very different from the fuels market and certainly very different from shopping for food at your local grocery store, but price has a very important influence on the supplier one chooses. With chemicals pricing, come other questions, such as: Is there a subsidy in the regional marketplace (as with ethanol in the USA)? What is the cost of alternative suppliers of feedstock(s)? What is the price to dispose or recycle any waste product? Is there a by-product that one has to also sell in order to get an attractive price for the targeted product? How energy intensive is it to produce the product; could it be produced using less energy? Is there a value to be gained by pursuing a green or more sustainable product, and how does one quantify that value? Does regional legislation impact the value/need for the product? What will the customers pay for that product; is there an upper limit?

If one looks at some SRI reports [3], one can get a feel for what factors contributes to the price of some chemicals. For example, in 2003, for a natural gas based H_2 plant [4] with a net production cost of 31.42 cents/hundred cu ft, the breakdown of the major cost contributors were natural gas, 22.32 cents (67.4%); catalyst 0.16 cents (0.48%); labor and supplies, 2.23 cents (6.7%); overhead, taxes and insurance, depreciation, and an allowance for general, administrative and other minor expenses, 8.38 cents (25.3%); and a utilities credit of 1.67 cents (5.3%). Again, this is only a very crude breakdown on relative production costs. Today's world scale H_2 plant is a major capital investment requiring many steps (feed purification, sometimes pre-reforming, steam generation, compression, steam reforming, gas recycle, secondary reforming, multiple heat recovery steps, steam recovery, water gas shift, gas separation by pressure swing adsorption, or perhaps a methanator, low temperature shift, a CO_2 stripper, and CO_2 adsorption [5]. People often forget about the extensive need for purification both in the front and back end because the catalysts or end user may require very low sulfur, CH_4, or CO levels in the product H_2 [6]. One has to be certain that any new process alternatives do not generate new or more impurities that would raise costs.

Looking at NH_3, the major production processes today are mostly based on the very old Haber–Bosch process using high pressure (>150 atm) N_2 and H_2 over a promoted iron catalyst at high temperatures. NH_3 plants are often considered to be H_2 plants because the production of pure, high pressure H_2 itself requires so much of the NH_3 plant equipment and has a significant impact on the cost of the NH_3 produced (remember 6 moles of H_2 for every mole of N_2). But to look at new routes to displace this long established technology, one has to look at other factors such as the cost of separating N_2 from air, compressing that N_2, producing the high pressure H_2 (often on-site), purification of the feeds, heating the reactor (>450 C), and separating and recovering the NH_3 (often by energy intensive refrigeration) from the product stream. Where new commercially applied catalysts have emerged (such as Ru/carbon) [7], not only is activity a factor, but also energy balance and reaction conditions. More recently, ammonia plants have been integrated with methanol plants, which necessitates changes in process design and demands large scale (for economy), a high demand, and often local use. A crude breakdown on manufacturing costs were natural gas, $54.06/tn; boiler feed water, 0.28/tn; cooling water circulation, $2.10/tn; catalyst cost, $1.7/tn; labor, $1.44/tn; supervision, $1.44/tn; interest, $1.30; indirect charges (capital, depreciation, insurance, maintenance, sales & marketing, etc.), $44.06/tn for a total cost of production of $106./tn (year 1990). While energy prices have a great influence on manufacturing costs, the actual selling price depends on supply and demand [8]. The manufacturing cost breakdown given above is mainly to see what goes into the cost of NH_3. It is highly influenced by the price of natural gas. For 15–20 years the price of natural gas bounced around $2.20/MMBTU, however in the past few years we have seen the price of natural gas spike (one spot price of $19/MMBTU) often due to its historical linkage to petroleum prices. [at $2.19/MMBtu, the cost of producing ammonia is about $100/ton; at $5.00/MMBtu, the production cost is about $200/ton (2003 estimates)] [9]. More recently, in the USA, the price of natural gas has taken a dramatic downward trend from world prices largely because increased domestic production and the optimism around huge deposits of shale gas in the USA [10,11]. So, with this example of NH_3, we see how complex the price for this commodity chemical can be influenced by the price of a fuel, since natural gas is also the feedstock to produce a non-carbon containing chemical. However, we cannot forget the impact of low catalyst costs in reducing capital investment, energy intensiveness, reduced operating conditions, transportation costs, and economies of scale.

4. Impact of the energy market

The availability and cost of energy has and will continue to have a significant impact on most chemical processes. Energy supplies around the world differ by regional resources and transportation costs. Worldwide, petroleum dominates the picture meeting about 35% of world energy demands, with coal ~25%, and natural gas ~20% [12]. The balance made up by nuclear, traditional biomass, hydroelectricity, and newer renewables (such as solar, wind, and biomass). Further, "energy" means one thing to a corporation and another to a residential customer. Again, what do we mean by the energy market? Actually, it comprises very diverse business sectors such as transportation, power generation, commercial, and residential customers. Huge, new reserves of shale gas in the US have and may continue to upset the oil/NG price ratio. Based on the end users, which varies considerably around the world, US transportation accounts for 28% and industry 32% of the consumption of energy [13]. In China industry accounts for 71% and transportation only 8% (but this is changing quickly). So, understanding the market, the customers, and where the product is being used have a big influence on "discovering" the next major energy advance, and that cost of energy will have a regional and global impact on the price and attractiveness of any chemical process.

What is impressive is the past and projected growth of the world's demand for energy. Over the last 30 years, all of the major fuel options have shown modest growth, but these growth rates are projected to increase significantly over the next 20 years. World energy demand is expect to expand by almost 45% between 2010 and 2030. It is clear that this demand is driven not only by sustained demand in the US and Europe, but by rapid growth in China, India, and other parts of Asia. In 2009, these 5 regions accounted for over 75% of the demand for crude oil, but demand does not match the resources. Today, the Middle East, Canada, South America, and Africa provide over 75% of the world's reserves of crude petroleum [14]. The key is that demand will remain tight and very susceptible to unpredictable events which can create havoc in the commodities market for petroleum and natural gas. When coupled with increasing populations, investor speculation, and people's natural quest to improve lifestyles, the price of oil, NG, chemicals, and energy will only go higher and higher.

The demands on energy supply will continue to push nations to retrieve dirtier sources of oil (such as oil shale and tar sands) and impure natural gas. Those market forces and environmental pressures, through tougher emissions controls and purification standards, will continue to drive new and substantial growth in purification methods and materials.

5. Tools for gathering market related information

A difficulty in gathering information of the value of new discoveries is that there is no readily available, single resource for understanding the shortcomings and limitations of most chemical processes. One often learns of those limitations, issues, and concerns by years of experience with specific products or by talking with experts. Obviously, one should try to get advice and guidance from multiple experts in a particular product area. One recent news story pointed to the value of university–industry "partnerships"[15] in understanding needs and shortcomings in the marketplace. In the absence of such close and open contacts, I suggest any of the following approaches – none of which is sufficient in itself – but represents a step forward in making a more credible assessment of the impact of one's research. This listing is not intended to be comprehensive, but does hit a number of excellent resources (in no particular order) for the catalyst/catalysis business and supporting the chemicals and petrochemicals industries.

- Look at trade journal magazines and searching their websites, such as: (a) Chemical Week, a weekly magazine on news and analyses of chemicals industries, published by IHS and on the www.chemicalweek.com; (b) Chemical Engineering Magazine (www.che.com); (c) ICIS Chemical Business—a weekly magazine providing an analysis of chemical markets, published by Reed Business Information Ltd at www.ICIS.com; (d) European Chemical News (www.europeanchemicalnews.com); (e) Chemical Marketing Reporter, www.chemicalmarketreporter.com.
- Conduct a thorough literature search on the process/product involved using a business oriented database.
- Read business specific technical publications, such as Hydrocarbon Processing, http://www.hydrocarbonprocessing.com/Magazine.html; Oil & Gas Journal, http://www.ogj.com/index.html; Nitrogen + Syngas, www.bcinsight.com; and Sulphur, www.bcinsight.com.
- Follow professional oriented magazines having technology sections, such as C&E News (published weekly by the American Chemical Society) http://pubs.acs.org/cen/, and Chemical Engineering Process (CEP) published monthly by the AIChE, www.aiche.org/cep.
- Review SRI Reports (now published by IHS) with a large portfolio of often excellent, specific product reports via their CEH program and PEP reports at www.SRIconsulting.com.
- Review reports from The Freedonia Group, www.freedoniagroup.com, which publishes market reports in a variety of technology areas.
- The Catalyst Group at www.catalystgrp.com.
- BCC Research, http://bccresearch.wordpress.com.
- Chemical Market Resources, Inc., http://cmrhoutex.com.
- There are also a number of small market research companies that do special assessments of some chemical products; these can often be found by doing a simple search on the World Wide Web.
- Chemical technology encyclopedias may often have some process, applications, and market information on major chemicals. Two such sources are the Kirk-Othmer Encyclopedia of Chemical Technology, published by John Wiley & Sons, Inc. and Ullmann's Encyclopedia of Industrial Chemistry, published by Wiley-VCH.
- Textbooks in applied catalysis, such as the excellent text and reference book by C. Bartholomew and R. Farrauto, Fundamentals of Industrial Catalytic Processes, 2nd edition, published by Wiley-Interscience, and Kent & Riegel's Handbook of Industrial Chemistry and Biotechnology, 11th edition, published by Springer.

6. Appreciating the impact

If you think that you have come up with some new catalyst or process, you need to find out if it really has some potential impact. It does not have to be immediate, but it is wrong to make an assessment that something has potential commercial value or it is a new process without seeking to verify in some manner whether the result has potential impact. I do not mean to define with numbers the market, but to at least talk with others who are experienced with the product area or the actual process and familiarize yourself with reports from some of the above resources (Section 5, above). If you cannot get help from those intimate with the production, talk to others who may have some limited knowledge. It is very important to establish the potential value of new discoveries before making claims about the commercial value or impact in the marketplace.

When considering the potential impact of a discovery, one needs to put it in context. For example, if you have discovered a catalyst that binds molecular nitrogen, it has little market value without being able to break the N–N bond, and a source of inexpensive hydrogen or hydrocarbon donor to make the ammonia or amine. In this specific example, the value is not in binding N_2, or making diimides, but getting to valuable products without spending a lot on materials or consuming large amounts of energy. It makes little sense to compete with today's established plants for making NH_3 from H_2 and N_2 if the hydrogen source becomes a very expensive hydride which could not be cost competitive for a large scale process requiring H_2. Importantly too, consider the energetics. Putting a lot of energy into making a product adds a cost which cannot be ignored. Then one has to consider separation demands, catalyst recycle, catalyst life, operating conditions required, cost and value of to address sustainability, etc. Catalyst life (stability) is often extremely important in operating a commercial process; assessing the life of a catalyst needs to be addressed over days of reaction not hours. While life studies over extended periods are needed in moving down a commercial pathway, what would be useful is getting a preliminary understanding of the extent and cause of catalyst deactivation early in the discovery process. The point is that there are often a lot of other considerations that go into a discovery that might offer potential to displace existing process routes.

As another example, consider that you have just discovered a material that absorbs CO_2. In this case, real value may come from what can you do with that absorbed CO_2. How much is absorbed per unit volume of material; is it reversible; how sensitive is the sorbed CO_2 to other components in a typical process stream (such as water vapor); and what are you going to do with the sorbed CO_2? If you going to reduce it—with what? Keep in mind that H_2 or even hydrocarbons are expensive sources of H-atoms. If you envision converting that CO_2 to a chemical, how much demand is there for that chemical and does it cost less to produce that chemical by existing routes than to fix and reduce the CO_2; how does the volume of the CO_2 contained in this material compare with the volume of CO_2 one seeks to reduce? A common mistake is to misunderstand the heart of the problem. For CO_2, a key issue is the huge quantities of dilute, impure (variable levels in a flue gas, presence of CO, CH_4, N_2, H_2O, etc.), low partial pressure CO_2 [13,16] produced by many different process gas streams; quantities so large that even converting some sizable fraction of the CO_2 to a chemical would only make a slight dent in the amount of global CO_2 emissions and saturate the global demand for the chemical being produced.

7. Using life cycle assessments, energy and mass balance operations

At some stage in any thorough analysis of a process, it may be helpful to do a mass and energy balance but also a Life Cycle Analysis (LCA) [17,18]. In addition, a sensitivity analysis [19] can be very useful in order to understand how various parameters in any process affect the results and which parameters are most critical to operations. The latter helps to focus the investigator on the true hurdles in moving a technology forward; a large number of scientists working on smaller, less critical hurdles needs to refocus around the major hurdles, not all taking them one step at a time.

A related example specific to CO_2 emissions comes from a recent mass balance/unit operations assessment on algae being used for biodiesel production, and serves as another example for being cautious and avoiding rash statements about the value of a research result. Kansas State University researchers working in agricultural economics and the Center for Sustainable Energy have reached some interesting conclusions [20] regarding the large-scale conversion of algae to biodiesel based on a careful mass balance analysis. Professor Peter Pfromm, said, “But while market conditions, prices and costs can be changed by tinkering with subsidies, mandates and policies, science ultimately cannot. . .Right now the fundamentals are the problem. It does not matter how well we engineer our production machine, the engine under the hood just is not that good,. . . The best option right now is to invest in fundamental research and design so that the yield can hopefully reach beyond the fifty grams per square meter per day on our most optimistic assumption.” These conclusions by Pfromm may not be widely shared and not acceptable to others, but they offer a platform from which to proceed to develop new information and results which might lead to a more attractive process.

8. Summary

Use the remarks within this manuscript to enhance your understanding and find value in your discovery. Certainly, not all research needs to be driven by a marketplace demand; there are very good reasons to pursue fundamental research, understanding mechanisms, catalyst characterization, as well as catalyst improvement and process optimization. My remarks are targeted at seeking to define the value of one’s discovery. For example, understanding diimide formation in activating N_2 does have value, but it needs to be placed in context. I [21] am just trying to encourage thinking around understanding the value of a discovery and avoid enthusiastic claims made about a discovery which stretches ones imagination and suggests a new or better process without really understanding much about the process or the hurdles in the marketplace.

There is a lot to gain by seeking to understand the dynamics of a chemical process, the marketplace around any new discovery and then understanding where that discovery offers value to the community at large or where it creates opportunities for high impact research. As these few examples above endeavor to illustrate, having made a discovery or an advance, try to determine its impact and avoid over-zealous statements about the value of the work by looking more closely at items such as total costs, energy and mass balance, all the process steps, the existing marketplace, etc. and then use all that to guide your work down the fundamentals or applied pathways.

References

[1] J. Armor, Ammoximation: I. A direct route to cyclohexanone oxime and caprolactam from NH_3, O_2, and cyclohexanone, J. Catal. 70 (1981) 72–83.

[2] J. Armor, Striving for catalytically green processes in the 21st century, Appl. Catal., A-Gen. 189 (1999) 153–162.

[3] The SRI home page provides a listing of available PEP reports at http://www.sriconsulting.com/PEP/ and CEH reports at http://www.sriconsulting.com/CEH/available_reports.html.

[4] PEP Yearbook, 2003, Process Economics Program, SRI Consulting.

[5] J. Armor, The multiple roles for catalysis in the production of H_2, Appl. Catal. A-Gen. 176 (1999) 161–178.

[6] J.N. Armor, Catalysis and the hydrogen economy, Catal. Lett. 101 (2005) 131.

[7] A. Ozaki, Development of alkali-promoted ruthenium as a novel catalyst for ammonia synthesis, Acc. Chem. Res. 14 (1) (1981) 16–21.

[8] T. Eggeman, in Ammonia, Kirk-Othmer Encyclopedia of Chemical Technology, Volume 2, John Wiley & Sons, Inc. Chapter available on line at http://www.scribd.com/doc/30120313/Ammonia.

[9] J. Sawyer, Natural gas prices impact nitrogen fertilizer costs, Integrated Crop Management, April 14, 2003; also at http://www.ipm.iastate.edu/ipm/icm/2003/4-14-2003/natgasn.html.

[10] G. Hess, Oil Shale Research is Moving Forward, C&E News, 2006 April 24, pp. 29.

[11] EIA report, Annual Energy Outlook for 2011, Report DOE/EIA-0383ER(2011).

[12] J. Goldemberg, Ethanol for a sustainable energy future, Science 315 (2007) 808–810.

[13] R. Smith, D. Dave, Carbon Capture from Coal Fired Power Generation, PEP Report No. 180B, SRI Consulting, December 2008.

[14] S. Davis, Crude Petroleum and Petroleum Products, SRI CEH Report, August 2010.

[15] P. Marie Morse, Rules of Engagement, C&E News, 2011 April 18, pp. 21–23.

[16] J. Armor, Catalytic fixation of CO_2: CO_2 purity and H_2 supply, in: T. Inui, M. Anpo, K. Izui, S. Yanagida, T. Yamaguchi (Eds.), Advances in Chemical Conversions for Mitigating Carbon Dioxide: Studies in Surface Science, vol. 114, 1998, p. 141.

[17] P. Holman, D. Shonnard, J. Holles, Using life cycle assessment to guide catalysis research, Ind. Eng. Chem. Res. 48 (2009) 6668–6674.

[18] P. Spath, M. Mann, Life Cycle Assessment of Hydrogen Production via Natural Gas Steam Reforming, DOE-NREL Report: NREL/TP-570-27637, February 2001.

[19] H. Song, U. Ozkan, Economic analysis of hydrogen production through a bioethanol steam reforming process: sensitivity analyses and cost estimations, Int. J. Hydrogen Energy 35 (2010) 127–134.

[20] P. Pfromm, V. Amanor-Boadu, R. Nelson, Sustainability of algae derived biodiesel: a mass balance approach, Bioresour. Technol. 102 (2011) 1185–1193.

[21] John Armor has worked in both academia (Assistant professor of inorganic chemistry, Boston University, 1970–1974) and in industry (Allied Chemical (now Honeywell, Inc) from 1974–1985 and Air Products & Chemicals from 1985–2004) since receiving his Ph.D. degree in chemistry in 1970 from Stanford University. He brings over 40 years of experience in catalysis (from homogeneous to heterogeneous) to his international consulting venture, GlobalCatalysis.com.