Technical & Commercial Progress in the Global Catalytic Process Industries

THE CATALYST REVIEW

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This Month's Special Feature

Progress in Technology for Polyolefin Production III

Industry Perspective: Where are we on the Open Innovation Journey?

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The Catalyst Group Resources, Inc. is a division of The Catalyst Group, Inc., a worldwide technical & commercial consultancy specializing in chemical process-driven change. The Catalyst Group Resources, Inc. is dedicated to helping clients understand the business impacts of technology change.

The Catalyst Review provides busy executives, researchers, and production managers with a timely update on catalysis and process advances in the petroleum, petrochemical, environmental, and specialty chemical industries.

More than 33 years ago ***The Catalyst Review*** was launched to fill an industry void: a highly-dense, digest-style publication aimed directly at corporate, R&D, academic and research science leaders in the $33 billion catalyst industry. It continues to accomplish this through its hand-selected experimental abstracts, in-depth company interviews, original “Special Feature” articles, expert perspectives, industry rumors, webinars and media reviews. This reinforces the purpose of ***The Catalyst Review***, which is to provide fresh news and research in a timely, easy-to-digest format. For more information, please call The Catalyst Group Resources (TCGR) at +1-215-628-4447, or email thecatalystreview@catalystgrp.com.

In This Issue

Where are we on the Open Innovation Journey?

A decade ago, most companies looked across the commercial landscape and realized that they have some great strengths and assets for selling and scaling products: brand, channels, manufacturing, product portfolios, and customer relationships. They also saw that the same organizational processes that drive profitable products are not well adapted for true innovation. A classic case of "The Innovator's Dilemma."

A generation ago big corporations were the natural owners of innovation: In the days of Bell Labs, DuPont's Central Research and others, successful technologies needed the infrastructure that the big companies could provide. It was hard to find the collaborators, the labs, and the ideas. The big corporate entity was instrumental to aggregating talent, capital, and research infrastructure to do great things. But no longer. With recent advances in software, flexible work and lab space, and widespread access to computing power and data storage for even the smallest companies, fundamental innovation can be the province of small enterprises and start-ups.

Out of these two trends *Open Innovation* was born. The promise was compelling: the creative power of a start-up partnered with the scale of an industrial Goliath. So how well are we doing with realizing that promise?

We are partway there. We have recognized the problem and challenge and gathered the will to address it. Many companies have done what they do well: stood up new organizations and allocated resources, both financial and human. They have created venture capital arms and Open Innovation hubs, hosted events, scanned the landscape for interesting companies, made connections, and provided input on countless panels. But much of the hard works remains: The work of real change. Change is hard. It's easier to tackle tactical activities than do the heavy lifting of organizational change.

I remain optimistic that the change is possible. There is a successful roadmap in the change that pharma undertook as it faced a similar innovation challenge a generation ago, eventually pivoting to partner extensively with biotech as an engine of innovation and growth. That pivot involved several changes that the Industrial sector, writ large, has yet to make:

1. Rethinking deals and partnering

In-licensing, development partnerships, and technology acquisitions are grooved in larger pharma companies and biotech companies and supported by knowledgeable bankers and consultants. Pharma started where industrials are now, with CVC often distant from the businesses and M&A teams grooved for asset transactions. It took years to develop the tools to assess and work with early stage companies, and even longer to recognize that strategic relationship management was a critical and unique skill, and often in short supply.

2. Setting aside old behaviors and mindsets

Mindsets are one of the hardest things to change. The attitudes and mindsets that got big enterprises to where they are now - because they are important in a battle between industrial titans - will not be the things that move them forward in a partnership mode. Recognizing and actively changing them are crucial. There are several that hamper Open Innovation collaborations: Not invented here syndrome, perfection and risk aversion versus bias for action, and win-lose (or risk shifting to the small entity) versus win-win for the partnership. Tackling these is hard, but necessary in order to capture the value of Open Innovation.

3. Redefining core competencies

In an Open Innovation setting, core competencies are different. It's no longer about control and expertise in all the processes from idea to product launch; it's about getting the best TEAM to collectively deliver excellence. To do that requires a rethink of core competencies are and how to deploy them in a team environment. Pharma ultimately learned that drug development, manufacturing, and clinical trial management were NOT the core competencies it wanted to control, despite that anyone 50 years ago would say that these tasks defined what a pharmaco was. Today's core competencies are process management, domain expertise, stakeholder networks, regulatory skill and marketing scale; each of which was a supporting expertise a generation ago.

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Egypt Implements $14Bln Refining, Petrochemical Projects...

Egypt is currently implementing a comprehensive programme for developing and modernizing the petroleum refining and petrochemicals sector through raising the efficiency of existing refineries and adding new production units, Minister of Petroleum and Mineral Resources Tarek El-Molla said. Work is underway for implementing five major petrochemical and refining projects with investments of about $14 billion, he revealed. The Chairman of Middle East Oil Refinery (Midor) said that the first phase of its expansion project which aims to boost the refining capacity to 60,000 barrels per day with investments of $2.4 billion will be complete in the upcoming period. The minister also followed up on the progress of Red Sea National Refining and Petrochemicals Company's $7.5 billion project, Anopc's $2.9 billion diesel production project with a capacity of 2.5 million tonnes per year, $64 million Asphalt project in Suez with a capacity of 1,200 tonnes per day, and $1.4 billion carbonisation complex in Suez. Source: Zawya, 8/5/2021.

Topsoe HydroFlex™ Being Used in Renewable Diesel Production at Phillips 66 Refinery...

In April, production of renewable diesel at Phillips 66's refinery in Rodeo, California, began, and Phillips 66 now reports successful start-up at the 9,000 barrels-per-day facility. With HydroFlex™, customers can convert low value feedstocks to renewable fuels that qualify for the California Low Carbon Fuel Standard (LCFS) credit. The innovative HydroFlex™ process layout offers lower capital expenditure (CAPEX), but also a lower energy consumption during operation, resulting in a lower Carbon Index (CI). Topsoe's HydroFlex™ can be deployed in both grassroots units and revamps for co-processing or stand-alone applications. The existing hydrotreater has the ability to produce renewable diesel from pretreated vegetable oils. Source: Haldor Topsoe, 8/10/2021.

Marathon Petroleum Produces 100 % Renewable Diesel...

Marathon Petroleum Corporation's Dickinson renewable diesel facility in North Dakota, USA has completed a successful test run of Haldor Topsoe's Hydroflex technology to produce 100 % renewable diesel. The technology helps to convert low-carbon renewable feedstocks into cleaner fuel alternatives. The new Hydroflex unit produces 100 % renewable diesel from soy and corn oil with a combined capacity of 12,000 barrels per day. The technology enables clients to convert low-carbon renewable feedstocks into cleaner fuel alternatives. Source: Process Worldwide, 8/6/2021.

Bapco Awards the Largest Catalyst Management Agreement in its History to ART for its Resid Hydrocracking Catalyst...

Advanced Refining Technologies LLC (ART), the joint venture of US specialty chemicals and materials company W. R. Grace & Co. and US energy company Chevron, announced the award of an full-cycle catalyst management (FCM) agreement by state-owned Bahrain Petroleum Company (Bapco). As part of the Bapco Modernization Programme (BMP), Bapco will boost Bahrain's oil refinery processing capacity from 267,000 (b/d) to 380,000 (b/d). In addition, ART will supply its Resid Hydrocracking catalyst technology for a wide variety of feedstocks to maximize bottom of the barrel upgrading. The technology is the industry-leading catalyst for metals capacity and sediment control. In addition, ART will provide FCM services for the reclamation of metals from spent catalysts. When fully operational in 2023, the new Resid Hydrocracking unit known as 1RHCU will be the main profit centre for the Bapco Refinery. 1RHCU utilizes LC-FINING process technology licensed from Chevron Lummus Global (CLG), a joint venture between Chevron and Lummus Technology. The unit is a two-train design with a processing capacity of 65,000 barrels per day. Source: W. R. Grace & Co., 8/11/2021.

KBR Awarded Ethylene Technology Contract by Hyundai Engineering and Técnicas Reunidas for PKN ORLEN Olefins Complex...

KBR announced that it has been awarded a technology licensing contract by Hyundai Engineering and Técnicas Reunidas for PKN ORLEN's Petrochemical Development Program in Plock, Poland. Under the terms of the contract, KBR will provide technology license, basic engineering design, and proprietary equipment for its leading ethylene technology, Selective Cracking Optimum Recovery (SCORE™), for PKN ORLEN's Olefins Complex III Project. This is Europe's largest petrochemical project in 20 years. KBR has licensed more than 100 grassroot ethylene plants utilizing its cost-effective and energy-efficient cracking technologies to produce ethylene, propylene and other valuable byproducts from a variety of feedstocks. Source: KBR, 8/9/2021.

BASF and SINOPEC to Further Expand Their Verbund Site in Nanjing, China...

BASF and SINOPEC will further expand their Verbund site operated by BASF-YPC Co., Ltd., a 50-50 joint venture of both companies in Nanjing, China. It includes the capacity expansion of several downstream chemical plants to support the growing Chinese market. The partners will expand the production capacities of propionic acid, propionic aldehyde, ethyleneamines, ethanolamines and purified ethylene oxide, and build a new tert-butyl acrylate plant. The tert-butyl acrylate plant will be an extension to the downstream using acrylic acid and isobutene of the existing Verbund as feedstock, which marks the first time this advanced production technology is applied outside of Germany. The expanded and new plants are planned to come on stream in 2023. Source: SINOPEC, 8/5/2021.

Haldor Topsoe and Yanchang Form Joint Venture and Build Methanol Catalyst Facility in China...

Haldor Topsoe and Shaanxi Yanchang Petroleum (Group) Co., Ltd. (Yanchang) formed a joint venture with the aim of delivering locally produced MK-151+ methanol synthesis catalysts to the Chinese market. Together, the two companies will build a production facility in Shaanxi Fupin in China to produce methanol synthesis catalysts. Topsoe and Yanchang have designed the plant and ordered long lead time equipment and therefore plan on starting up beginning of 2022. Forming of the joint venture and building of the catalysts facility will be the first step of a long-term strategic cooperation between Topsoe and Yanchang. Source: Haldor Topsoe, 7/28/2021.

PBF Energy Selects Honeywell Technology for Potential Renewable Diesel Fuel Project...

Honeywell announced that PBF Energy Inc. would use Honeywell Ecofining™ technology for a potential renewable diesel project at its Chalmette Refinery in Louisiana. The process produces Honeywell Green Diesel™ fuel, which is chemically identical to petroleum-based diesel and can be used as a drop-in replacement in vehicles with no engine modifications. Depending on feedstock choice, renewable diesel also features up to an 80% lifecycle reduction in greenhouse gas emissions compared with conventional diesel. The U.S. Environmental Protection Agency's Renewable Fuel Standard program requires all domestic oil refineries to blend renewable fuels into the diesel pool to reduce greenhouse gas emissions, which also expands the domestic fuel supply. PBF is currently evaluating the conversion of an idle hydrocracking unit at the plant to a single-stage Ecofining unit that if built would produce 20,000 barrels per day of renewable diesel fuel. Source: Honeywell UOP, 8/5/2021.

Maire Tecnimont Group Awarded €130 MN Petrochemical Contract by Kazanorgsintez PJSC in the Russian Federation...

Maire Tecnimont S.p.A. announces that its subsidiaries Tecnimont Planung & Industrieanlagenbau GmbH and MT Russia LLC have been awarded by Kazanorgsintez PJSC (KOS) an EP contract (Engineering and Procurement) for the execution of a Low-Density Polyethylene (LDPE)/ Ethylene-Vinyl Acetate (EVA) plant, to be implemented inside the existing KOS facilities, located in Kazan, in the Republic of Tatarstan (Russian Federation). The scope of the project includes the implementation of a new LDPE/EVA Plant with a capacity of 100,000 tons per year. The Project will be mainly aimed at expanding the production capacity of polyolefins, and its completion is expected within about 40 months from the contract signing date. The portion of the scope of work in the Russian Federation will be performed by MT Russia in its Moscow engineering centre, where Maire Tecnimont Group employs about 200 specialists currently involved in several ongoing Russian projects. Tecnimont Planung & Industrieanlagenbau is Tecnimont's German engineering subsidiary located in Braunschweig, highly specialized in the design of LDPE plants. Source: Maire Tecnimont, 8/5/2021.

India's Reliance Eyes More than Doubling of PET Recycling Capacity...

Indian conglomerate Reliance Industries Limited (RIL) will more than double its polyethylene terephthalate (PET) recycling capacity by setting up a recycled polyester staple fiber (PSF) manufacturing facility in Andhra Pradesh. Srichakra Ecotex produces recycled PSF and recycled hollow conjugate fibre, both of which are produced from post-consumer PET bottles. It is a subsidiary of Telangana-based Srichakra Polyplast, an end-to-end recycling and plastic waste management company that produces R-PET and recycled polyolefin granules. The new plant will help RIL to more than double its recycling capacity to 5bn post-consumer PET bottles. RIL currently converts more than 2bn post-consumer PET bottles into fibres annually. RIL currently recycles PET bottles at plants at Barabanki in Uttar Pradesh state, Hoshiarpur in Punjab state and Nagothane in Maharashtra state. Source: ICIS Chemical Business, 8/5/2021.

BioTfueL® Project: Entry Into the Industrialization and Commercialization Phase...

Bionext and its partners have successfully completed the test program on BioTfueL® demonstration units, a crucial step in the development of this technology that will allow the production of low carbon footprint biokerosene. This demonstration made it possible to validate, develop and optimize the process chain on a semi-industrial scale on 4 different types of biomass after 1000 hours of gasification and more than 1500 hours of torrefaction. Based on the experimental results obtained, the partners are already hard at work to industrialize the BioTfueL® technology with a view to its commercialization in early 2022. This is an important step aimed at positioning BioTfueL® technology as the great option to produce Sustainable Aviation Fuels (SAF) allowing to reduce GHG emissions by more than 90%. BioTfueL® technology will contribute by its deployment to the achievement of the SAF incorporation targets set by the French State in 2020 and proposed by the European Commission in 2021 in its «fit for 55» package, which is 5% in 2030 and more than 50% by 2050. Each BioTfueL® industrial unit would allow the production of 30 to 100 kt/year of SAF and would create several hundred agricultural, forestry and industrial jobs. Source: IFP Energies Nouvelles, 8/2/2021.

KBR and Petron Scientech Inc. Sign Alliance Agreement to License Sustainable Technologies...

KBR and Petron Scientech Inc. (PSI) announced that they have signed an alliance agreement to license differentiated, energy-efficient, and sustainable technologies for renewable chemicals production. Under this agreement, KBR will be the exclusive licensor for PSI's Ethylene Oxide / Ethylene Glycol (K-MEG℠), Alcohol Dehydration (K-SEET℠) and Maleic Anhydride (Max-Leic℠) technologies, which are used to convert ethanol into ethylene and further derivative chemicals used in a wide range of industry and consumer products. KBR will license these technologies and provide engineering services for new biorefineries as well as integrating the technologies in existing refineries and petrochemical plants to offer sustainable alternatives. Source: KBR, 8/3/2021.

BASF, Eni Partner to Develop Advanced Bio-Propanol Production Technology...

Eni and BASF have signed a strategic agreement on a joint R&D initiative to reduce the CO_2 footprint of the transportation sector. The cooperation aims to develop a new technology to produce advanced bio-propanol from glycerin, a side stream of the production of industrial biodiesel (FAME, fatty acid methyl ester), that Eni will purchase from European producers. The technology under development involves the conversion of glycerin to propanol via an innovative, catalytic hydrotreatment process. The new approach consists of a process of applying a high-pressure hydrogenation reaction over a BASF catalyst, ensuring that the bio-propanol is produced with a high yield and purity while minimizing by-products. The bio-propanol offers the potential to reduce GHG emissions by 65 to 75% compared to fossil fuels. Source: BASF, 7/29/2021.

OOO Zapsibneftekhim to Use Honeywell Technology to Increase Polymer-Grade Propylene Production...

Honeywell announced OOO ZapSibNeftekhim, a subsidiary of PJSC Sibur Holding, will revamp one of its facilities in western Siberia that uses Honeywell UOP C_3 Oleflex™ technology to increase propylene production. The revamp will enable the Russian company to increase production of propylene by more than 8%, to 561,000 metric tons per year, to meet the growing demand for propylene derivates used in polymer production. UOP provides technology licensing and basic engineering design, in addition to services, equipment, catalysts and adsorbents for the unit. Honeywell UOP's C_3 Oleflex technology converts propane to propylene through catalytic dehydrogenation. Global production capacity of propylene from Oleflex technology currently stands at approximately 10.2 million metric tons per year. Source: Honeywell UOP, 8/4/2021.

Johnson Matthey and Kebotix in Partnership for AI-Enabled R&D Projects...

Johnson Matthey and Kebotix, a U.S.-based technology platform company for new chemicals and materials, announced an agreement to explore developing the next generation of coatings for catalytic converters. The project will support JM's digital strategy and help to bring the company to the forefront of digital R&D. Kebotix's lab-of-the-future AI capabilities has the potential to enhance JM's digital transformation in the chemical industry. The collaboration will seek to discover innovative methods to increase the efficiency of experiments leading to the optimisation of catalytic converter coating formulations. Scientists can use the predictions as a virtual catalyst design lab and validate their design choices to avoid spending unnecessary experimental resources on suboptimal designs. The project will employ Kebotix's ChemOS Pro technology, developing machine learning models via the company's proprietary active learning optimisation algorithms. Source: Chemical Engineering, 8/4/2021.

Sabic, ExxonMobil Announce Major Milestone for JV...

ExxonMobil and Sabic said that their joint venture, Gulf Coast Growth Ventures (GCGV) located near Corpus Christi in the US state of Texas, has reached mechanical completion of a monoethylene glycol unit and two polyethylene units. The project, which includes a 1.8 million metric ton ethane steam cracker, is expected to be delivered under budget and approximately 25% less than the average cost of similar projects along the US Gulf Coast. When completed, GCGV will produce 1,100 kilotons of monoethylene glycol and 1,300 kilotons of polyethylene per year. Ownership interests in the Gulf Coast Growth Ventures project is 50% ExxonMobil and 50% Sabic. Project startup is expected to begin ahead of schedule, likely in the fourth quarter of 2021, a Sabic statement said. Source: TradeArabia, 7/28/2021.

FlexCat™ by Unifrax Produces Increased Yield with Less Coking in Model PDH Study...

Unifrax announced initial results of the first phase of its testing campaign, performed at hte GmbH. FlexCat™, a new customizable fiber-based catalyst support material, is designed for use in industrial catalysis, improving the output of hydrogen and specialty gas production, chemical processing, air purification and other chemical manufacturing applications. FlexCat™ increased output by 20% in the initial cycle and retained at least 90% conversion activity during the subsequent cycle tested. This patented technology provided more tortuosity, maximizing catalyst interaction and producing 50% less side products per cycle, including four times less benzene. Source: Business Wire, 7/27/2021.

Jiangsu Sailboat Petrochemical Co. Ltd. Selected LyondellBasell's Lupotech T Technology...

LyondellBasell announced that Jiangsu Sailboat Petrochemical Co. Ltd. will use again LyondellBasell Lupotech T high-pressure polyethylene technology at their facility located in Lianyungang City, Jiangsu Province, P.R. of China. The process technology will be used for a 200 KTA ethylene vinyl acetate copolymer (EVA) and low-density polyethylene (LDPE) line to produce EVA products with vinyl acetate comonomer. Decades of experience in high-pressure application design makes the Lupotech T process one of the preferred technologies for EVA/LDPE plant operators. High reliability, unmatched conversion rates and effective process heat integration are key attributes of the Lupotech T process, designed to ensure this technology's on-going energy efficiency. More than 13 MIL mt/yr of Lupotech T EVA/LDPE production capacity has been licensed by LyondellBasell in over 70 lines around the world. Source: LyondellBasell, 7/27/2021.

Clariant Expands its Capacity for Emission Control Catalysts to Meet Growing Demand...

Clariant Catalysts is expanding and enhancing its capacity for emission control catalysts to meet growing global demand, particularly in China. The company just recently commenced operations at an additional, upgraded production facility in Heufeld, Germany, which features state-of-the-art production equipment exclusively dedicated to emission control catalysts. The catalysts are suitable for off-gas abatement in a diverse range of applications, from chemical production plants to stationary engines and turbines. The EnviCat® range includes catalysts for the removal of various harmful emissions, including volatile organic compounds (VOCs), hydrocarbons, carbon monoxide, nitrous oxide, nitrogen oxide, and ammonia. Production capacity for the catalysts has been increased to enable a volume growth of 100% compared to 2019. Source: Clariant, 7/26/2021.

Chandra Asri Secures $1.3B for Second Indonesian Petrochemical Complex...

After a long wait, plans are now moving forward toward a final investment decision on Indonesia's second ethylene center, CAP2. A large chunk of funds here will be coming from PTT PCL group company Thai Oil PCL, which is set to acquire 15 percent of new shares to be issued in CAP2 project leader PT Chandra Asri Petrochemical Tbk. for up to $914 million. On top of this investment will be $400 million coming from a chemical subsidiary of the Siam Cement Group (SCG), as well as an additional $400 million coming from these two companies subject to the final investment decision. While all of this is not yet enough to match the total estimated investment amount of $5 billion, the financing provided here by Thai Oil and SCG has at least given the project the driving force needed toward the final investment decision that is scheduled for next year. Investment here will also be a major boon for the project's ability to secure feedstock naphtha, which in Indonesia is typically imported. In coming on board with the project, Thai Oil will supply approximately 1.05 million tons of naphtha and natural gas per year as feedstock for CAP2 and Indonesia's existing ethylene center, CAP. Then in addition to this feedstock supply deal, Thai Oil has secured the right to distribute approximately 176,000 tons per year of polyethylene and polypropylene – along with roughly 124,000 tons per year of aromatics – produced at CAP and CAP2. Meanwhile, SCG – already a major shareholder in Chandra Asri – will be offered share purchase rights to maintain its 30 percent-plus ownership stake in the Indonesian company. Source: Japan Chemical Daily, 8/5/2021.

Scientists Set their Sights on New Catalyst Technology to Help Achieve Net Zero...

A partnership featuring two leading British universities, Cardiff University and The University of Manchester, together with bp and Johnson Matthey (JM), has been launched to explore transforming carbon dioxide, waste products and sustainable biomass into fuels and products that can be used across the energy and transportation sectors. The project is one of eight business-led Prosperity Partnerships announced in support of the UK government's ambitious new Innovation Strategy. Cardiff University, an internationally-leading centre for catalysis research, is leading the project, and The University of Manchester will provide expertise in materials science, characterisation methods and catalysis. They are joined by bp, which is transitioning from an international oil company to an integrated energy company, and Johnson Matthey, a global leader in sustainable technologies. The partnership will devote the next five years to exploring new catalyst technology to help the world get to net zero. Commencing in October 2021, the work brings together industry experts from bp and JM with academics from Cardiff University and The University of Manchester in this interdisciplinary team. Source: Johnson Matthey, 7/22/2021.

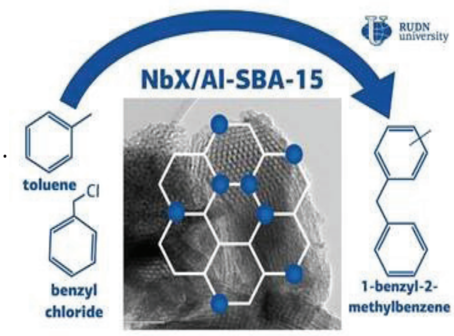
Less is More: "Reduction" Allows for Cleaner and More Efficient Catalytic Reactions...

In an ongoing effort to accelerate catalytic reactions, oxidation of metal complexes using light has emerged as a standard method to synthesize aromatic compounds. Now, researchers at Tokyo Institute of Technology have demonstrated a high-yield synthesis pathway through reduction of rhodium complexes, using a newly designed catalyst that enables electron-deficient elements to be added to aromatic compounds, opening up possibilities to synthesize bioactive products and functional materials.

In a new study published in the Journal of the American Chemical Society, researchers from Tokyo Institute of Technology (Tokyo Tech) have expanded the scope of light-induced metal-catalyzed reactions by demonstrating a synthesis method that uses an "anionic" (negatively charged) Rh complex to enable the addition of an electron-deficient boron group to an arene. In their study, they used a newly designed cyclopentadienyl (Cp)-rhodium-based catalyst, which initially formed a neutral complex with the arene. This complex then underwent a "reduction" (gain of electrons) under light irradiation to form an anionic intermediate that, in turn, facilitated an exchange of a ligand (a molecule attached to a metal atom) with a diboron group to yield compounds called "arylboronates" in a process known as "borylation. After testing a variety of catalysts on arenes and the diboron group, they found that the neutral metal complex had to be excited to a "triplet state" with light, before it could be reduced to its anionic state to yield the corresponding arylboronate. The new synthesis strategy worked for arenes containing a wide variety of functional groups and generated high yields (up to 99%). Furthermore, compared to the conventional metal-catalyzed borylation, it used milder reactants and allowed borylation at room temperature, making the process cleaner and more energy-efficient. Source: Tokyo Institute of Technology, 8/11/2021.

A Chemist from RUDN University Synthesized a Silica and Niobium-Based Catalyst to Speed Up Petrochemical Reactions 24 Times...

A chemist from RUDN University found a way to speed up alkylation reactions to 24 times. To do so, he developed a catalyst based on silica and niobium. For the process to go on quickly and efficiently, it needs catalysts including mineral acids and zeolites—minerals that are capable of selectively releasing substances and then adsorbing them back. A chemist from RUDN University created a catalyst that is free from microporous disadvantages and able to speed up the alkylation reaction up to 24 times. To do so, his team used niobium and SBA-15, a mesoporous ordered form of silica. The team paid attention to the reductive-oxidative and acidic properties of niobium-based compounds that are important for a catalyst and decided to test niobium in an alkylation reaction. To do so, they put niobium oxide nanoparticles (that had been mechanochemically ground down to several nanometers in size) on the support. The metal content in the new material varied from 0.5% to 1% and the size of the particles was controlled with a transmission electron microscope. To analyze the catalytic properties of the new material, the chemists carried out the reaction of toluene alkylation with benzyl alcohol and benzyl chloride that acted as alkylating agents. As a result of the experiment, the team confirmed a positive effect of niobium particles on the reaction: its time of reaction reduced from 4 hours to 10 minutes. The catalyst with lower niobium content (0.5%) turned out to be more effective due to better dispersion. The team believes that when the catalyst was synthesized, niobium oxide deposited on the support, and the more niobium, the bigger the catalyst particles turned out to be. This reduced the effective contact area of the particles and therefore had a negative impact on the material's catalytic activity. Source: RUDN University, 8/3/2021.



Scientists Led by NTU Singapore Identify New Catalysts for More Efficient Water Splitting...

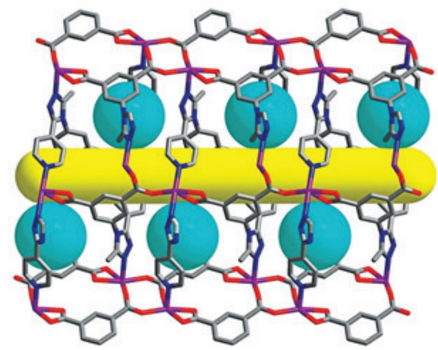
A team of scientists led by Nanyang Technological University, Singapore (NTU Singapore) have discovered the parameters that determine the efficiency of a class of low-cost catalysts called spinel oxides – a discovery that breaks a bottleneck in the extraction of hydrogen from water through electrolysis, the process of splitting water with electricity. NTU Singapore's Associate Professor Jason Xu Zhichuan and his team have made two important advances. They have unravelled, at the atomic scale, how spinel oxides work to speed up water electrolysis. Primed with that new understanding, the team then used machine learning to select new spinel oxides with increased catalytic activity, making water electrolysis more efficient. Assoc. Prof. Xu, who is also part of NTU's Energy Research Institute, said the main bottleneck lies in the chemical reaction that leads to oxygen generation from the other side known as the oxygen revolution reaction. Based on key parameters that the team had identified the team trained a machine learning model with a dataset of over 300 spinel oxides in order to screen and predict the efficiency of any spinel oxide catalyst in a matter of seconds. Using this method, the team found that a new oxide comprising manganese and aluminium was predicted to show superior catalytic activity. This was validated experimentally. The NTU-led team was supported by researchers from institutes in Beijing and Hong Kong, in addition to those from Agency for Science, Technology and Research (A*Star) and National University of Singapore. The work is funded by the Ministry of Education and the National Research Foundation. Source: Nanyang Technological University, 8/3/2021.

Bottling Clean Energy in Chemical Bonds...

A team led by chemist and laboratory fellow Tom Autrey is working to turn chemical energy storage into practical setups that could one day help power neighborhoods, infrastructure, and industry. Research at the PNNL's Energy Sciences Center will include work focused on developing new catalysts for converting electricity into chemical bonds through the Center for Molecular Electrocatalysis. Autrey and the team are developing hydrogen carrier systems that harness chemical reactions to add and remove hydrogen from stable molecules on demand. An entire subfield of chemistry studies the catalysts that perform hydrogen addition and removal. PNNL researchers specialize in designing catalysts that facilitate storing hydrogen in molecules such as formic acid, methylcyclohexane, and butanediol, among others. PNNL chemist Ba Tran led work testing the suitability of hydrogen-rich ethanol, combined with an established catalyst, to cycle with ethyl acetate for long term storage. Hydrogen remains bonded to the ethanol until needed, when it can be released for use and the ethanol converted into ethyl acetate. The catalyst can add two molecules of hydrogen to a single ethyl acetate molecule, producing two stable ethanol molecules that store the hydrogens. In addition, Tran and his colleagues incorporated data from experimental measurements and advanced molecular simulations into studies of larger-scale systems. "We want to see how the process of storing hydrogen in ethanol—and other forms of chemical energy storage—would behave in an application-scale system," said theoretical chemist Samantha Johnson. Source: Pacific Northwest National Laboratory (PNNL), 7/26/2021.

MOF Sieves Propylene from Propane...

Scientists have explored using metal-organic frameworks (MOFs) to separate propylene from propane. Researchers at Jinan University now report a MOF that can sieve 99.5% pure propylene from a 50-50 mix of propylene and propane in a single pass. Chemists led by Weigang Lu and Dan Li invented the MOF, known as JNU-3a. It features a slim channel with a series of small, orthogonal pockets—like a long, straight hallway that has many rooms coming off it. These pockets are dynamic and will sequester either propylene or propane, depending on how much pressure the MOF is under. To separate the propylene and propane, the researchers flow the hydrocarbons through JNU-3a at 1 kPa of pressure. Propylene gets trapped in the pockets while propane flows through. The researchers then purge the MOF to get 99.5% pure propylene. JNU-3a can be readily recycled and reused by flowing helium through the material. Source: Chemical & Engineering News (C&EN), 7/26/2021, p.11.



This illustration of JNU-3a shows the MOF's central channel in yellow and orthogonal pockets in teal. Gray = C, red = O, blue = N, purple = Co. Credit: Adapted from Nature

Industry Perspectives continued from page 1

4. Defining Ownership and Simplifying Processes

While large organizations can muster tremendous resources, ownership can often be opaque, and decision making slow. Who has input? Decision making power? Who needs to be syndicated with? What can the organization do and not do? What can it commit? In the context of an established partnership, this can slow the execution, value creation and de-risking that the partnership was designed to create.

Simplifying decision making for an Open Innovation model is critical to capturing the nimbleness, speed and de-risking that underlie start-up innovations. Locking innovation in a corporate process designed for more established products is not a recipe for success. This often means pushing decision making lower (or less centrally) in the organization and risking moving forward 10 steps and back 1, rather than forward only 2. Simple decisions should be simple.

I remain a fervent believer in the combination of start-up engines and industrial titans as a force for bringing innovation and value to industry, customers, and the world. I am optimistic and hopeful we can get there.

About the Author

Erica Nemser is the CEO of Compact Membrane Systems, a pioneer in industrial separations. She was formerly a consultant with McKinsey & Company in the pharmaceutical sector. She looks forward to hearing your stories of success and triumph as well as your challenges and setbacks. Feel free to reach Erica at enemser@compactmembrane.com

Progress in Technology for Polyolefin Production III

By Eugene F. McInerney, PhD

Introduction

For almost 40 years, The Catalyst Group Resources (TCGR) has published a multi-client study series on advanced polyolefin catalysts, processes, and products. Based on TCGR's groundbreaking 2011 study, "Progress in Technology for Polyolefin Production: Quantifying the Valued-Added of Advanced Catalysts, Co-Catalysts/Activators, and Stereo Regulators," and two more focused updates in 2017 and 2018 (i.e., "Polyolefin Catalysts and Processes: Technological and Commercial Impacts on PE and PP" and "Polyolefins Catalysts and Processes: Competitive Implications of Industry Consolidation"), it was time for a more in-depth and comprehensive industry reassessment.

In this 2020 update (***"Progress in Technology for Polyolefins Production III"***), TCGR revisits both the new product markets and the R&D pipelines, documenting and analyzing opportunities of benefit to polyolefins (PO) producers in their business planning decision making. A key addition to this new study is a comprehensive "Voice of Customer Survey" involving resin converters and the changing resin requirements to meet future needs. In addition, it documents, via patent and literature surveys, detailed assessments of emerging technologies, as well as product and process advances, including:

- New and improved PO resins to serve the faster growing differentiated or "specialty" market applications, including large volume price-sensitive markets, as well as sophisticated niche applications.
- Gains in production volumes from fixed assets can be achieved through recent improvements in processes and catalysts, co-catalysts/activators, and/or electron donor (ED) technologies.
- Value-added returns on R&D, which can result from developing, licensing, or joint venture cutting-edge polyolefin process, catalyst, co-catalyst/activator, and product advances.

Herein, the authors summarize this comprehensive industry reassessment but recommend that those readers interested in acquiring a greater depth of perspective can visit the webpage dedicated to the report, including the actual TofC at https://www.catalystgrp.com/multiclient_studies/progress-in-technology-for-polyolefins-production-iii/, or by contacting Chris R. Dziedziak at +1.215.628.4447 or cdziedziak@catalystgrp.com.

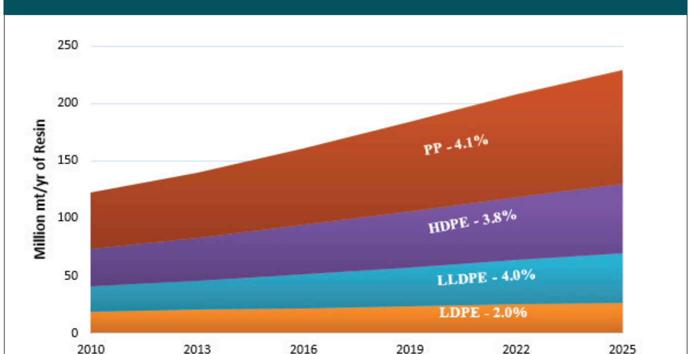
Beginning with a treatment of Economic Concerns, the author will then discuss Recent Developments in Polyolefin Catalysts and Processes before discussing the results of Voice of Customer/Survey of Converter's Needs followed by TCGR's Recommendations and Conclusions.

Economic Concerns

Supply and Demand

COVID-19 dramatically impacted both the actual and the forecasted supply and demand for polyolefin resin and catalysts. China is the leading consumer, followed closely by North America and Europe. Film and sheet applications are the largest end-use. North America and the Middle East will remain as export heavy regions, with China increasing their overall petrochemical self-sufficiency over the coming decade. **Figure 1** reflects the demand for polyolefin resin production, LDPE, LLDPE, HDPE, and PP-forecasts for 2020 and beyond had the COVID-19 pandemic never taken place. LLDPE accounted for about 32% of PE resin demand and was forecasted to grow by around 4% globally out until 2025. China is the largest consumer of LLDPE and will likely continue to be. It will increase capacity in the coming years, along with the US and other parts of Asia; however, it will still be dependent on imports. HDPE accounted for about 46% of PE resin demand and was forecasted to grow just under 4% globally until 2025. Asia,

Figure 1. Polyolefin resin growth since 2010 (and 2019-2025 CAGR).



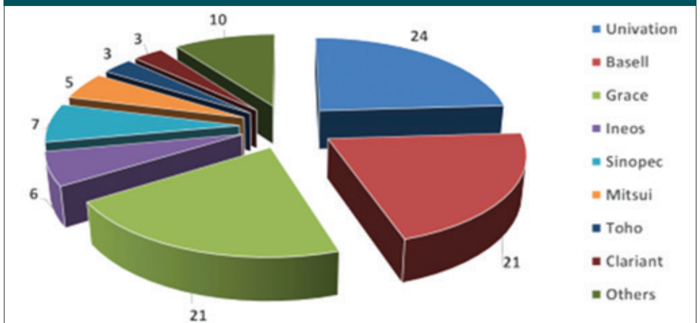
Source: TCGR, 2020a

driven by China, is the largest consumption and production region, with North America a distant second. North America is expected to continue to be a net exporter, and Europe will likely be a net importer as it deals with capacity reductions. Most of the world's planned polyethylene (PE) capacity additions are for either LLDPE or HDPE, at least before 2020. For 2019-2021, most of these additions are in China, the United States, Russia, and other parts of South East Asia.

Of the four different polyolefin resins, polypropylene is the single largest volume resin, with global production reaching more than 77 mil mt in 2019. It was also projected to grow at 4.1% CAGR until 2025, the fastest of the four. Early in 2020, when the COVID-19 pandemic was beginning to hit the Western world, projections were that overall polypropylene (PP) demand could be anywhere from 2 to 4 mil mt lower since PP demand would likely suffer a greater negative impact compared to PE. However, IHS Markit has revised some of their initial projections and has put demand growth at around 0.6%. Much of this may be due to China, which has had a good economic recovery compared to many other countries. PP demand in China may have even grown close to 10% compared to 2019, which, according to ICIS, brings the global growth up to 2% (ICIS, 2020).

Along with resin demand and growth are the respective fresh catalyst production for each resin type. The total polyethylene catalyst market was valued at close to $1.3 bil USD in 2019 by TCGR and is expected to grow around 4% annually out to 2025 (TCGR, 2020a). The total polypropylene catalyst market was valued at nearly $1 bil USD, growing around 4.4%. The following pie chart (**Figure 2**) depicts the leading PE and PP catalyst producers. In summary, COVID-19 has dramatically impacted both the actual and the forecasted supply and demand for polyolefin resin and catalysts.

Figure 2. PE/PP catalysts 2019 global market shares (USD %).



Source: TCGR, 2020a

Specific growth rates, by polymer/resin, include:

- LDPE accounts for about 22% of all PE resin demand and is typically forecasted to grow around 2-3% annually (globally) but was projected to inch closer to 2% as we move out to 2025.
- LLDPE accounted for about 32% of PE resin demand and was forecasted to grow by around 4% globally out until 2025.
- HDPE accounted for about 46% of PE resin demand and was forecasted to grow just under 4% globally until 2025.
- PP is the single largest volume resin, with global production reaching more than 77 mil mt in 2019. It was also projected to grow at 4.1% CAGR until 2025, the fastest of the four.

Market Drivers

Some of the main market drivers in the short term will all revolve around COVID-19. The chemical and plastics industries have been impacted differently, and COVID-19 has positively and/or negatively affected many businesses over the last year. Early in the second quarter of 2020, consumers flocked to buy home goods, groceries, and hand sanitizer, among other items sought to be essential at that time. The food and restaurant industry has had to adjust, offering more takeout options and less dining on-site. Due to government-enforced lockdowns and quarantines, many people found themselves at home, inspired to purchase household goods and cleaners and improve their homes, leading to high demand for home improvement and independent recreation. In the United States, low down payment and low-interest rate loans have spurred home buying growth and home construction. And of course, medical supplies and personal protective equipment will continue to be in high demand both now and into the foreseeable future. Lastly, the purchase of online goods through companies like Amazon.com is at an all-time high, increasing the demand for packaging materials. Packaging companies and converters will be driven to create cost-effective but more sustainable and lightweight packaging. Plastics play a major role in all these areas, and short-term demand for them will continue to be positive well into 2021. However, industries like automotive and air travel, and thus the required plastics to support them, have been negatively impacted and will take longer to recover.

Another key market driver both now and in the future is the recycling of plastics. The public will continue to pressure governments and chemical and polymer companies to utilize more recycled plastics, if not reduce or find alternatives to plastics altogether. Plastics will continue to serve a major role in the global economy. Much attention will be paid to utilizing more recycled feedstocks, improving mechanical and chemical recycling methods, investing in new recycling plants, and designing regulations and laws that improve plastics' overall recycling. Many companies have declared sustainability goals due to pressure from the public, investors, or governments to reduce their greenhouse gas footprint and/or lowering the carbon intensity of the products they sell. Companies in the polyolefins industry will address this global dilemma by incorporating recycled feedstocks, offering products that are partially or wholly comprised of recycled polymers. They will also reduce the complexity of individual products to allow for easier recyclability while designing advanced catalytic and thermal solutions to make products that are easier to separate and recycle. Additional market drivers that will impact the polyolefins industry include:

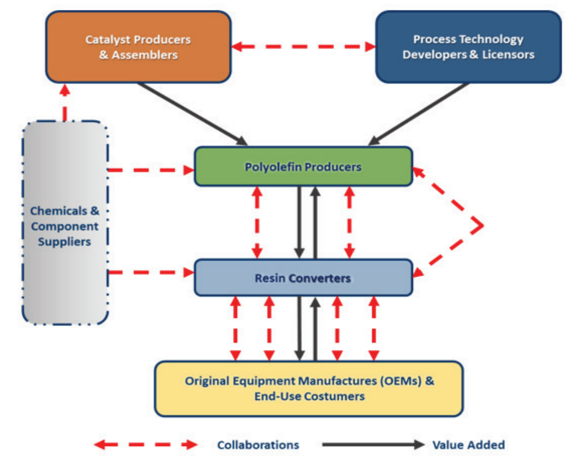
- Increasing usage of plastics in automotive applications to improve fuel economy. Fuel economy standards will likely continue to become more and more strict. Electric vehicles will require different solutions than traditional combustion vehicles as well.
- In addition to recycled plastics, bio-resins will continue to gain traction as an alternative way to address sustainability. Like recycled plastics, this is driven by consumer/public pressure.
- Reinforced plastics
- Automation, 3D printing, Industry 4.0

Regulatory Impacts

In December 2015, the European Commission adopted an EU Action Plan for a circular economy. It identified plastics as a key priority and prepared a strategy addressing plastics' challenges throughout the value chain (**Figure 3**) and their entire life cycle. The regulatory pressure, commitment to using incremental amounts of recycled plastics in their produced goods, and the 2018 China ban on polymer waste import have contributed to global environmental concern surrounding polyolefins production (TCGR, 2020b).

A proposal to restrict four phthalates commonly found in plasticized materials was prepared in 2016 by the European Chemicals Agency and Denmark due to the toxicity found in finished product plastics. As of 2018, the enacted requirements of REACH (Registration, Evaluation, Authorization, and Restriction) now restricts the four phthalates listed in the **Table 1** (QIMA, 2019).

Figure 3. The polyolefin value chain.



Source: TCGR, 2020b

At one point, most PP catalysts in the industry were 4th generation catalysts, which was a global concern many years ago, and 4th generation catalyst producers and manufacturers were under tremendous regulatory pressure to evaluate alternatives in polypropylene production. The restrictions of phthalates in finished products have impacted polyolefin production, and it has created manufacturers to seek catalysis alternatives. The generations of Ziegler-Natta Catalysts shown in **Table 2** have given rise to the increasing presence of toxic phthalates in plastic-a fact that has driven and directed polypropylene research to develop new materials for these catalysts.

Table 1. Types of phthalates.

Item	Acronym	Name	Maximum Concentration (ppm)
1	BBP	Butylbenzyl phthalate	0.1%
2	DBP	Di-n-butyl phthalate	0.1%
3	DEHP	Bis(2-ethylhexyl) phthalate, (Di(2-ethylhexyl) phthalate)	0.1%
4	DIBP	Diisobutyl phthalate	0.1%

Source: QIMA, 2019

Many regulations have been the drivers in the fifth and sixth generations moving away from phthalates or reducing their content. The general push from many consortiums and government agencies has led to revamping the Ziegler-Natta catalysis to produce polypropylene. However, it is not merely regulation that drives the stepwise improvement of $TiCl_3$ based Ziegler–Natta catalyst technology to 5th and 6th generations of catalysis. New catalysts such as metallocene/methylaluminoxanes (MAO) will allow for the synthesis of polymers with highly defined microstructure, tactility, stereoregularity, and long-chain branched, or blocky copolymers possessing excellent properties.

Table 2. Generations of Ziegler-Natta Catalysts.

Generation	Base	Internal donor	Activating Agent	External donor
1st	$TiCl_3$ and $AlCl_3$	None	DEAC	None
2nd	$TiCl_3$ and $AlCl_3$	None	DEAC	None
3rd	$TiCl_4$ and $MgCl_2$	Benzoate	TEAL	Benzoate
4th	$TiCl_4$ and $MgCl_2$	Phthalate	TEAL	Silane
5th	$TiCl_4$ and $MgCl_2$	Diether	TEAL	Silane (although not always necessary)
	$TiCl_4$ and $MgCl_2$	Succinate	TEAL	Silane
6th	Zirconocene	Uncertain	MAO	Uncertain

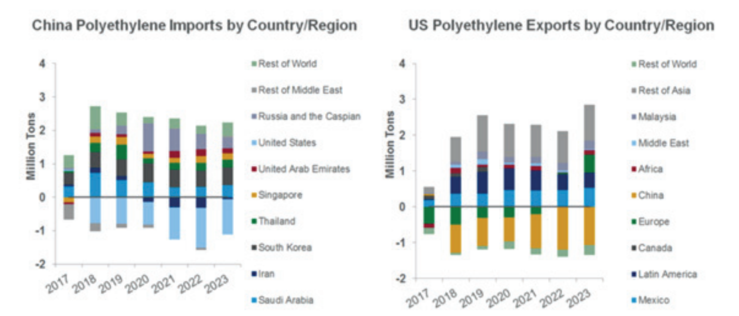
DEAC= diethyl aluminum chloride, TEAL= triethyl aluminum, MAO= methylaluminoxane

Source: AMEC, 2013

Trade Dynamics

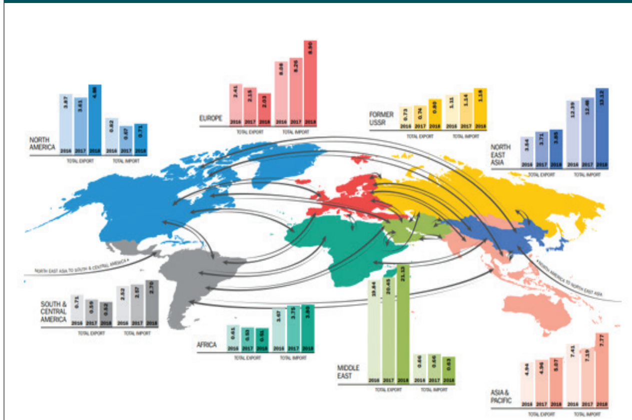
Increasing shale gas availability in the US will lead to more significant exports of PE. China will continue to add polyolefin production capacity but will continue to be a major importer in the near term, with many Asian exports from the Middle East. The US and the Middle East will likely compete for exports to both Asia and the Middle East, but this will continue to be complicated by the US/China trade tariffs. There are expectations that a change in presidential leadership in the US will ease these tensions, but political implications will be affected beyond this report's scope. The above comments can be applied to both PE and PP. See **Figure 4** and **Figure 5** for information on global polyolefin trade flows.

Figure 4. China/US polyethylene imports and exports, by country/region.



Source: Wood Mackenzie, 2018

Figure 5. Worldwide polyolefin trade flows (in million metric tons).



Source: ICIS, 2017

Recent Developments in Polyolefin Catalysts and Processes

This subject area constitutes the heart of ***Progress in Technology for Polyolefins Production III: Voice of the Customer Driving Innovation and Growth in Polyolefins Catalyst and Process Technologies***, and contains a detailed examination of patents and commercial literature-by year, by company, by region, and separated by polyethylene (PE) catalyst, polypropylene (PP) catalyst, PE process, and PP process- reveals numerous vital advances.

First and foremost, the identity of the companies conducting most of the patenting is noteworthy, with process licensors lagging somewhat behind resin producers. Also, the areas of focus were broadened beyond catalysts and processes to include co-catalysts, activators, supports, operating conditions, and even post-reactor resin modifications and separations. Lastly, the leading developers continue to focus on two critical challenges/opportunities: (1) approaches towards higher productivity/lower costs; and (2) approaches towards new/improved resin properties/performance.

A synopsis of the catalyst/process technology developments for PE and PP includes:

- In terms of regional shifts in the catalyst industry, China has emerged as a new source of PO catalysts and catalyst technologies, and Saudi Arabia is emerging as a new source of catalysts and technologies (both pro-catalysts and co-catalysts). South Korea will follow shortly.
- R&D in the polyolefins value chain is dynamic, and in some areas, it is currently more fruitful than it has been for almost three decades.
- Industry research efforts cover the full spectrum of traditional Ziegler-Natta and chromium oxide catalysts through advanced single-site catalysts. from traditional free radical high pressure polymerized LDPE to unique new elastomeric polyolefins with structures controlled on a nanoscale.
- On average, about 30% of innovations flowing from industry R&D can will result in new business growth for the owners built on new platform technology.
- Another 25% hold promise for the future following further development.
- The remaining 45% offer incremental competitive advantages built on established technology platforms.
- Of the total number of developments reviewed: 56% related to catalysis, 30% related to products and their applications, 14% related to process applications. Moreover, 40% of all developments reviewed involved metallocenes or other single-site catalysts; and 20% of product developments related to specialties, with the remaining divided equally between PE and PP, approaches towards new/improved resin properties/performance.

Catalysis is the most essential aspect of industry research efforts: Major breakthroughs are being made to reduce metallocene/SSC costs and expand their versatility. Complex catalyst systems are being developed to simultaneously control multiple product characteristics, such as MWD, composition distribution, and molecular branching structure. These are targeted at “single-reactor bimodal” process technologies, mainly for PE, but PP is a target also. These bimetallic systems include chromium oxide systems, Z-N systems, and particularly metallocene systems. Metallocene and SSC systems are targeted at producing new types of elastomer with property profiles never available. Demand for these elastomers is expected to grow strongly. SSCs are being applied to the production of new-to-the-market polymer modifiers that are significantly increasing the range and combinations of properties available in PE and PP products. These modifiers have high value, justifying premiums.

The advances in process technology made or claimed by leading licensors or key producers have been noteworthy. Areas of focus have been on the key process technologies, such as UNIPOL, MARTECH, Borstar, Hyperzone, etc. Tremendous progress continues to be made in three (3) key areas: in improving the effectiveness and versatility of catalysts, in the production of improved products, and in reducing manufacturing costs.

The value chain starts with catalyst suppliers and ends with the final end-users, as represented by converters who satisfy these end-users’ needs. The potential to add incremental value through R&D and innovation varies over a wide range from tens of thousands of dollars per ton for catalyst producers down to single-digit dollars per ton for licensors.

Of the total value created by innovation, 25% flows to the investor or developer, and 75% flows to other downstream stakeholders – seems to give reasonable estimates of value allocation. The value domain within which each stakeholder operates limits the dimensions of value creation in terms of differential premium per ton or kilogram of product. The value domain is defined as the difference between raw materials costs and product selling price. Examples of stakeholders include catalyst producers, process licensors, PO resin producers, and resin converters. The potential value created by innovation in PO products derived quantifications indicating likely price premiums for advantaged products. Advanced catalysts should be worth an extremely high premium because of the high degree of leverage. Enhanced process technologies may justify increases in process royalties. Thus, there is substantial value creation potential in recent technology developments.

Voice of Customer/Survey of Converter’s Needs

The “voice of customer” surveys with producers in the plastics industry document how some recent macro trends and issues affect their business and product development work. Additionally, they indicate how the resin converters currently perceive recent advances in polyolefins technology and what sort of advances are desired in the future. Ten companies provided valuable input on their business’s key issues and what they would like to see from the future’s polyolefins industry. These companies included the following: Performance Pipe, Pipeline Plastics, LLC, Central Plastics, Inc., Allied Plastics, Inc., Plastics UNLIMITED, C-P Flexible Packaging, Berry Plastics Corporation, Myers Industries, Inc., and Transcendia, plus one additional resin producer, ESENTTIA). Selected highlights include:

- Technology advances are recognized by some but not all resin converters, which seems somewhat dependent on the applications each convertor serves. For example, converters serving the PE pipe industry have appreciated the improvements in crack and abrasion resistance. However, many states that P65 rather than P100 still seems to be the bulk of demand. There is still innovation and perhaps consolidation to come.
- The film industry views metallocene PE as being superior. There has been a trend to move from several tie layers (3-4) towards 6-7 layers to improve barrier resistances and impart special features. Non-phthalate Z/N catalyst resins are recognized by some converters servicing the food packaging industry. However, other convertors outside this application have no focus on this as being an immediate concern.
- For PP converters, the major areas of interest are low VOC improvements, needed as a priority being requested by the automotive manufacturers for internal parts. Newer PP products with higher MW and bimodals for improved strength favor cost/performance resins. BOPP has found important niches but has not seen the same product growth rates that were earlier anticipated. While homogeneous non-isotactic PP has historically been an important ingredient in the CASE market, elastomers’ growth is taking a greater role.
- All converters are focused on sustainability to a certain extent. Although converters were aware of the single-use plastic issue, many of those interviewed did not seem significant. Convertors were more acutely aware of the need to make products more recyclable using single polymer packaging. Also, the need to use more post-consumer recycled plastics was a growing trend and should focus on the polyolefins industry in the future.

Recommendations and Conclusions

The thermoplastics sector remains a high-growth area, and polyolefins, as the largest segment, have long-term attractiveness. However, there are numerous challenges yet to be addressed; the potential of the shifting negative impact on the growth of the virgin resin production demand because of polyolefins circularity due to recycling and development as well as the deployment of new cost-effective solutions to chemicals recycling. Catalysis and compatibilization will lead to higher-value industry solutions. A selection of key recommendations and conclusions includes:

- The trend towards plastics circularity and recycling is real. Producers who secure their supply/demand in fruitful market applications proactively will fare better than those who do not.
- There are still significant gains in production productivity through improved catalysts and automated process controls. Targeted R&D will reward investors with higher ROIs.
- Developing catalysts with improved internal and external donors and activators has proven to be a winning combination across various producers and catalyst company advances to improve activity, reduce cost, and tailor product properties.

Lastly, TCGR concludes that clients using this study will be able to view developments between producers rather than merely internally, seeking out these trends and providing access to essential benchmarks to internal producers' R&D programs to attain a competitive advantage.

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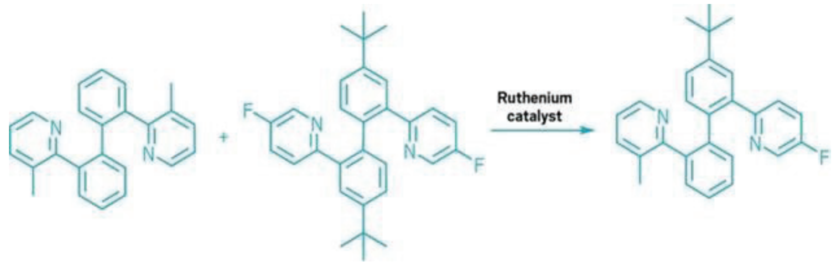
About the Author

Dr. Eugene F. McInerney received his doctorate in organometallic chemistry from St. John's University (NY). As a 60-year member of the American Chemical Society, he has been involved in various technological challenges and innovations in such diverse fields as photocatalysis, semiconductor fabrication, polymer synthesis and fabrication, composite materials, and alternate energy systems. His professional experience includes corporate roles in business and market development, international licensing, program management, mergers and acquisitions, and strategic planning. For the past 20 years, he has applied his skills to assist emerging companies in achieving sustainability. Since 2009 he has served as a contributor to the "Experimental" and "Movers & Shakers" sections of *The Catalyst Review* and can be reached at www.linkedin.com/in/eugenefmcinerney.

C-C Single Carbon Bonds in Familiar Way…

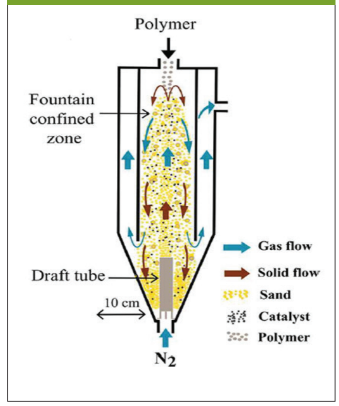
Guangbin Dong and coworkers at the University of Chicago have uncovered a metathesis reaction that not only works with single-bonded biaryl rings but is reversible. Although alkane metathesis reactions are known, Dong says, either they involve olefin formation or they are not reversible. Here, the group synthesized a series of compounds with two of the same aryl groups, then used a ruthenium catalyst to create biaryl compounds with two different aryl groups (shown). Chemists previously would have used a cross-coupling reaction that required an oxidant or reductant, or an acid or base. Dong's method works with many functional groups, including rarely tolerated bromides and boronates, and does not need redox or pH-adjusted conditions. It's more simple and straightforward, Dong says. "You just add a catalyst, then the bonds break and re-form." Through computational analysis, the team found that the reaction goes through an "olefin-metathesis-like" pathway, Dong says, in which the compound breaks a C–C bond to oxidatively add to the catalyst. A reductive elimination then forms the new C–C bond. This research shows that direct C–C single-bond metathesis is possible, which is potentially useful, Dong says. Source: Chemical & Engineering News (C&EN), 8/9/2021, p.13.



Conversion of HDPE into Value Products by Fast Pyrolysis Using FCC Spent Catalysts in a Fountain Confined Conical Spouted Bed Reactor…

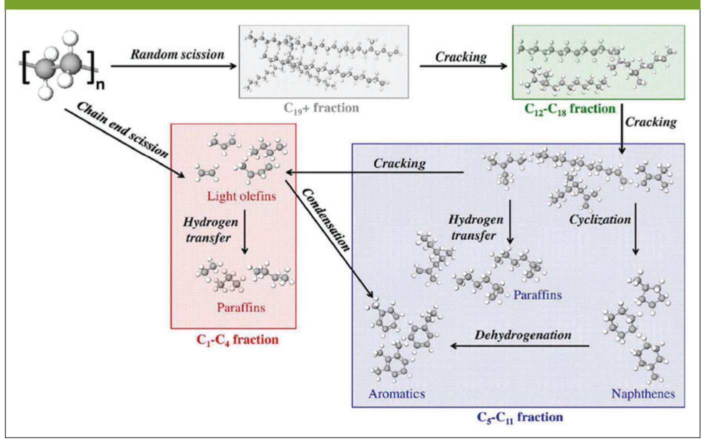
In 2018, the European Commission established a specific strategic plan for plastics, in which guidelines were given for producing, using, and recycling plastics. Mechanical recycling is the most common procedure for plastic management. However, this process often causes final product quality problems due to the thermal and mechanical degradation undergone by the material. An alternative strategy involves using thermochemical conversion technologies, which allow producing fuels and high value-added chemicals. Herein, the authors describe the use of a conical spouted bed reactor (CSBR) provided with a draft tube and fountain confiner (**Figure 1**) for the catalytic pyrolysis of high-density polyethylene (HDPE). The reaction is carried out over a spent fluid catalytic cracking (FCC) catalyst composed of HY zeolite (16 wt%) and various additives, such as silica, alumina, and clay. These workers found that the use of the CSBR allows for continuous plastic feed without defluidization problems and is especially suitable for catalytic pyrolysis with high catalyst efficiency. The main product fraction obtained in the catalytic cracking was made up of C_5-C_{11} hydrocarbons, with olefins being the main components. The yield decreased as temperature and residence time were increased due to reactions involving cracking, hydrogen transfer, cyclization, and aromatization.

Figure 1. Gas and solid flow circulation in a fountain confined CSBR provided with a non-porous draft tube in the plastic pyrolysis.



Catalytic pyrolysis of HDPE occurs through the following general steps: (i) polymer melting; (ii) coating of catalyst particles with fused plastic; (iii) fused plastic pyrolysis; and (iv) catalytic cracking of fused plastic and pyrolysis volatiles. Secondary reactions in the gas phase may also occur in the waste plastics catalytic pyrolysis, although the conditions attained in the CSBR (i.e., short residence times, high heating rates, and relatively low reaction temperatures) limit the extent of these secondary reactions. The cracking steps involving the molten HDPE (**Figure 2**) are thought to involve a random scission mechanism to yield long-chain hydrocarbons or via end-chain scission to yield lighter hydrocarbons. The former pathway is the main pathway of thermal cracking and leads to waxes – the primary HDPE pyrolysis products.

Figure 2. Main reaction pathways in HDPE catalytic cracking.



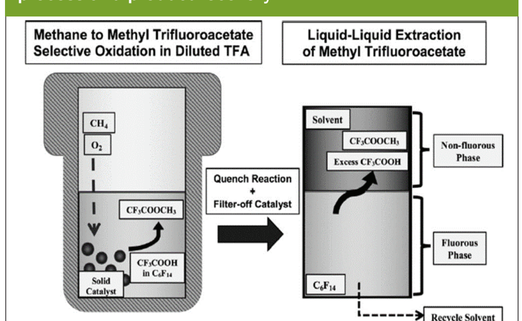
The authors conclude that the catalytic activity of the spent FCC catalyst for HDPE cracking has now been demonstrated and that the yield of waxes (thermal cracking primary products) is negligible above 550°C. Moreover, the obtained products have significant commercial value, as is the case of light olefins, especially propylene and butenes, and liquid fuels in the range of gasoline and diesel. Source: Orozco S, Artetxe M, Lopez G, et al. (2021). ChemSusChem, doi.org/10.1002/cssc.202100889.

Heterogeneously Catalyzed Aerobic Oxidation of Methane to a Methyl Derivative…

Although well-established industrial routes for methane utilization exist, they tend to be energy and capital-intensive processes. As such, they are economically unviable for methane valorization at small- and mid-scale facilities, such as remote and decentralized shale oil production sites. Consequently, efforts to develop a more scale-flexible direct methane conversion route have motivated both the academic and industrial communities. Herein, the authors present an aerobic methane-to-methyl-ester approach that utilizes a highly dispersed, cobalt-containing solid catalyst, possessing significantly more favorable reaction conditions compared to existing homogeneously catalyzed processes.

Several homogeneous transition metal-based catalysts display activity for methane to methyl trifluoroacetate conversion, including those based on copper, manganese, and cobalt. Therefore, these workers set about to synthesize a variety of transition metals on solid supports that were then screened for activity in a batch reactor system (**Figure 1**). Based on their initial screening results, cobalt-containing silica catalysts synthesized via an incipient wetness impregnation (Co/SiO_2-IWI) with an

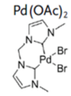
Figure 1. Overview of designed methane oxidation process and product recovery.



The conversion of methane to methyl trifluoroacetate occurs in an autoclave charged with methane, air, solid catalyst, and a solution of TFA in perfluorohexane. After reaction, methyl trifluoroacetate is extracted from the fluorous reaction medium into a nonfluorous solvent.

aqueous cobalt nitrate solution showed the most promising activity. **Table 1** lists the Co/SiO_2-IWI catalyst activity with known homogeneous catalytic systems that oxidize methane to methyl trifluoroacetate. The use of a fluorous co-solvent as an acid diluent provides several advantages, notably a milder reaction environment that allowed working in a heterogeneous mode and a facile product and solvent recovery method through a highly effective extraction with a non-fluorous solvent.

Table 1: A comparison to homogeneous systems for the oxidation of methane to methyl trifluoroacetate.

Entry	Pre-catalyst	Oxidant	$P_{methane}$ [bar]	Reported TO[a]	Productivity[b] [$mol_{ester}\ mol_{metal}^{-1}\ h^{-1}$]	Ref.
1	$Pd(OAc)_2$	$K_2S_2O_8$	20	3.8	0.2	[18]
2		$K_2S_2O_8$	30	30	2.1	[18]
3	$H_5PV_2Mo_{10}O_{40}$	$K_2S_2O_8$	10	128[c]	6.4[c]	[19]
4	CuO	$K_2S_2O_8$	5	33	1.9	[11c]
5	$Co(OCOCF_3)_3$	O_2	20	4	1	[20]
6	$EuCl_3$/Zn	O_2	10	5.3	5.3	[21]
7	$FeCl_3$	O_2	10	<0.5	<0.5	[21]
8	$Pd(OAc)_2$/BQ/$H_5PMo_{10}V_2O_{40}$	O_2	25	3–118[d]	0.4–14.8[d]	[22]
9	$Co(OAc)_2.4H_2O$	O_2	20	13.2	0.6	[23]
10	Mn_2O_3	O_2	7	8.5	2.8	[11b]
11	$[Pd(hfacac)_2]$	H_2O_2	30	39	9.8	[24]
12	$[Cu(hfacac)_2(H_2O)_2]$	H_2O_2	30	13	3.3	[24]
13	$VO(acac)_2$	H_2O_2	50	18.5[c]	0.8[c]	[25]
14	$H_4PV_1Mo_{11}O_{40}$	H_2O_2	50	224[c]	9.3[c]	[25]
15	0.1% Co/SiO_2-IWI	O_2	5	31	10.3	This study

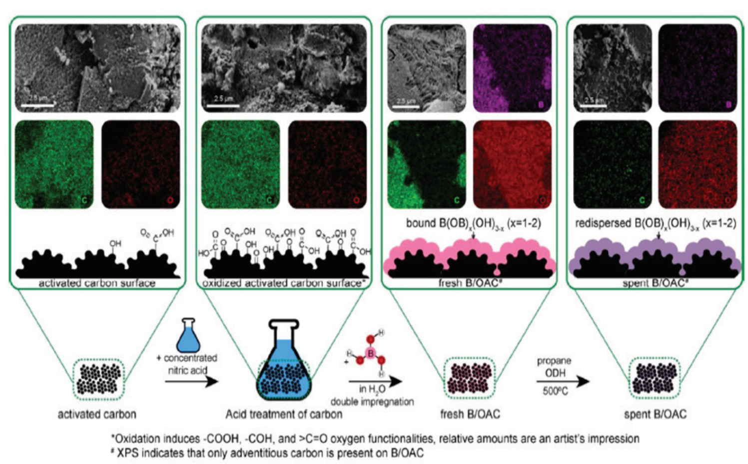
[a] [Moles of methyl trifluoroacetate]/ [Moles of metal in catalyst] measured over the reported reaction time; [b] Average rate of production based on reported metal/catalyst loading and reaction time; [c] Including methyl acetate as a product; [d] Determined with respect to $Pd(OAc)_2$.

The performance of these systems was compared based on the reported turnovers (TO) over the reaction period and productivity. Reported turnovers reported typically represent a lower bound on the amount of product formed per mole of catalyst since, in most cases, it appears that the catalyst may not be fully deactivated at the end of the reaction period. The Co/SiO_2-IWI catalyst achieved turnovers of up to 31 and a corresponding productivity of 10.3 $mol_{ester}\ mol_{Co}^{-1}\ h^{-1}$. The performance is competitive to even homogeneous systems that employ more potent oxidants ($K_2S_2O_8$, H_2O_2), higher partial pressures of methane, and/or more complex redox cycling schemes. This data illustrates the outstanding catalytic performance of the system that is achieved with an economical oxidant and under reaction conditions that are more favorable than those generally employed in state-of-the-art methane-to-methyl-ester systems. Source: Blankenship AN, Ravi M, Newton MA, et al. (2021). Angew. Chem. Int. Ed., doi.org/10.1002/anie.202104153.

Highly Selective Carbon-Supported Boron for Oxidative Dehydrogenation of Propane…

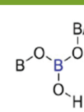
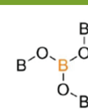
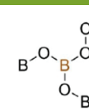
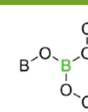
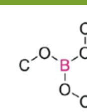
Boron-containing materials are highly effective for the oxidative dehydrogenation (ODH) of light alkanes to light olefins. In particular, bulk and nanotubular hexagonal boron nitride (h-BN) exhibits high selectivity towards propylene for the ODH of propane. Investigation of oxidized/hydrolyzed boron oxide species used for ODH has been carried out via the synthesis and characterization of silica-supported boron oxide materials (B/SiO_2). Detailed characterization of B/SiO_2 ODH catalysts has shown that most of the boron is composed of clustered 3-coordinate boron oxide/ hydroxide species [$B_2(OH)_{2x}O_{3-x}$, x=0– 3]. Additional studies have suggested that an improved supported boron catalyst should 1) stabilize dispersed oxide/ hydroxide species and 2) not feature an exposed hydrophilic surface as silica. Herein, the authors explore the use of activated carbon, treated with nitric acid, and impregnated with boric acid as a boron source referred to as B/OAC (**Figure 1**).

Figure 1. Schematic illustration for the synthesis of the B/OAC catalyst and SEM/EDX microscopy of the denoted carbon sample.



The synthesized B/OAC catalyst yielded excellent selectivity towards propylene. It was found to be the most selective supported boron catalyst reported thus far, exhibiting nearly the same product distribution as h-BN. Furthermore, B/OAC is significantly cheaper than h-BN, potentially making it more economically viable. Reactivity data indicated that B/OAC did not experience support interactions that result in reduced selectivity, as in B/SiO_2, likely due to a boron overlayer stabilizing and coating the carbon support. Molecular-level characterization through XPS, IR, Raman, and solid-state NMR spectroscopies revealed that the B/OAC

Table 1. Boron speciation and populations[a] determined by solid-state NMR spectroscopy.

Boron Species[b]					
δ_{iso} (ppm)[c]	18.3	17.0	15.0	13.6	11.5
Fresh Population (%)	60	19	7	12	2
Spent Population (%)	51	17	11	15	6

[a] Populations were determined from the quantiative (recyle delay > $5\times T_1$) 10° tip-angle single pulse spectra. [b] The color of the highlighted boron atom corresponds to the color of the analyitical fits given in Figure 5. [c] All boron species have C_Q = 2.65 MHz and η = 0.

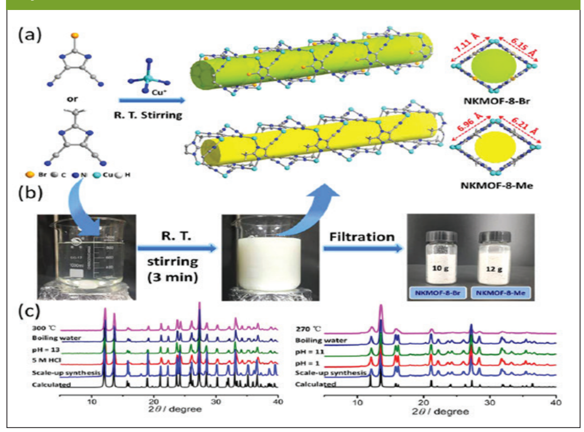
material under atmospheric conditions contains clustered oxidized/ hydrolyzed boron species residing on the surface of the carbon support. Spectroscopic analysis of B/OAC before and after catalysis reveals minimal differences, suggesting that while the boron structure may change under reaction conditions, the material reverts to its initial state upon removal of heat and reactants.

Furthermore, 2D ^{11}B MQMAS solid-state NMR spectra of the fresh and spent catalysts revealed five unique boron species: $B(OB)_x(OH)_{3-x}$ (x=1–2), $B(OB)_3$, $B(OB)_2(OC)$, $B(OB)(OC)_2$ and B $(OC)_3$. (**Table 1**). Analytical fits of quantitative ^{11}B solid-state NMR spectra illustrated that $B(OB)_x(OH)_{3-x}$ (x=1–2) and $B(OB)_3$ species make up ca. 80% of all boron, confirming that most of the boron is clustered on the surface of the carbon support. Source: Mark LO, Dorn RW, McDermott WP, et al. (2021). ChemCatChem, doi.org/10.1002/cctc.202100759.

Scalable Room-Temperature Synthesis of Highly Robust Ethane-Selective Metal−Organic Frameworks for Efficient Ethylene Purification…

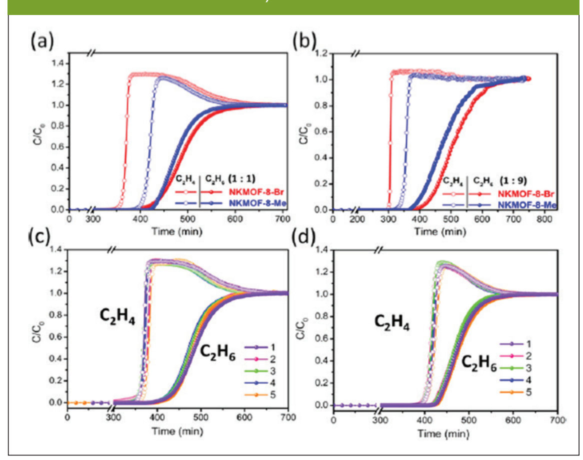
Ethylene is typically produced via the cracking of hydrocarbons, but it must be free of ethane to be commercially valuable. Purification is usually performed in a large distillation tower (120−180 trays) under energy-intensive and high-cost conditions (low temperature and high pressure). Adsorption-based separation techniques have attracted increasing attention, especially those using adsorbents such as metal-organic frameworks (MOFs). These materials are characterized by their high efficiency, easy operation, and low energy consumption. However, the separation of ethylene and ethane is extremely challenging due to their similar physical properties and molecular size. In addition, the presence of ambient water vapor further complicates the issue since water often acts as a competitor for binding sites. Herein, the authors describe the design, synthesis, and evaluation of two new C_2H_6-selective MOF adsorbents (NKMOF-8-Br and -Me) capable of capturing C_2 hydrocarbon gases at ambient conditions even in high humidity.

Figure 1. (a) Synthetic routes and structures of NKMOF-8-Br and -Me. (b) Demonstration of the large-scale synthesis of NKMOF-8-Br (10 g) and -Me (12 g). (c) PXRD patterns of NKMOF-8-Br (left) and -Me (right) after various treatments and large-scale synthesis.



Metal−organic building blocks without open metal sites (e.g., tetrahedral MN4 building blocks, M = Cu^+, Zn^{2+}, and Co^{2+}) and nonpolar/inert pore surfaces (e.g., small, conjugated ligands) were selected for the construction of C_2H_6-selective adsorbents. The reaction of two aromatic imidazole derivative ligands with Cu+ ions afforded two new C_2H_6-selective MOF adsorbents, NKMOF-8-Br and -Me (**Figure 1**). These two isostructural MOFs possess a regular ultra-microporous 3D pts network and exhibited remarkably high stability against harsh treatments such as boiling water, acid/base, or heating at 300°C. The nonpolar pore environments and appropriate pore apertures enabled the preferential adsorption of C_2H_6 over C_2H_4. Thus, NKMOF-8-Br and -Me possessed high C_2H_6/C_2H_4 selectivity and C_2H_6 uptake, surpassing most reported C_2H_6-selective MOFs.

Figure 2. (a) Experimental breakthrough curves of the C_2H_6/ C_2H_4 (1:1, v/v) mixture with He as the carrier gas (70%, vol %) for NKMOF-8-Br and -Me at 298 K and 1 bar. The total flow rate was 3 mL/min. (b) Experimental breakthrough curves of a C_2H_6/ C_2H_4 (1:9, v/v) mixture with He as the carrier gas (70%, vol %) for NKMOF-8-Br and -Me at 298 K and 1 bar. The total flow rate was 3 mL/min. (c,d) Five cycles of experimental breakthrough curves of the C_2H_6/C_2H_4 (1:1, v/v) mixture with He as the carrier gas (70%, vol %) for NKMOF-8-Br and -Me at 298 K and 1 bar. The total flow rate was 3 mL/min.



Confirmation of the separation performance was carried out by conducting breakthrough experiments of NKMOF-8-Br and -Me using a C_2H_6/C_2H_4 (1:1, v/v) mixture with He as the carrier gas (70%, vol %). By purging this mixture into a packed column with a total inlet flow rate of 3.0 mL/min at 298 K, the C_2H_6/C_2H_4 separation was achieved using the NKMOF-8 MOFs (**Figure 2a**). To further evaluate the performance of NKMOFs, breakthrough experiments were conducted with NKMOF-8-Br and -Me for a C_2H_6/ C_2H_4 (1:9, v/v) mixture with He as the carrier gas (70%, vol %) (total flow rate 3.0 mL/min, 298 K). Using NKMOF-8-Br and -Me, C_2H_4, which passed first through the packed column, was detected in the outlet gas with a purity of >99.99%. After 85 and 60 min, respectively, C_2H_6 was eluted through the packed column (**Figure 2b**). NKMOF-8-Br and -Me exhibited excellent regeneration and reusability. It was found that NKMOF-8-Br and -Me could be recycled for at least five cycles in a dynamic C_2H_6/C_2H_4 column breakthrough test without any deterioration in separation performance (**Figure 2c, 2d**). Source: Geng S, Lin E, Li X, et al. (2021). J. Am. Chem. Soc., 143: 8654−8660.

Danielle Ballivet-Tkatchenko, Dr.h.c.

CNRS Honorary Senior Researcher

Danielle Ballivet-Tkatchenko was awarded a Doctorate in Physical Sciences from the University of Lyon, France, in 1970. As a CNRS research fellow, she developed her independent career successively at Institute of Research on Catalysis and the Environment of Lyon (IRCELYON, Villeurbanne), Laboratoire de Chimie de Coordination (LCC Toulouse), and Institut de Chimie Moléculaire de l'Université de Bourgogne (ICMUB, Dijon). Her research interests focus on designing ever more challenging active and selective catalysts having potential industrial interest for making chemicals/fuels through sustainable routes. Danielle was awarded Doctor honoris causa from the University of Oulu, Finland, for her contribution in the field of CO_2 utilization. She chaired the 11th International Conference on Carbon Dioxide Utilization in 2011 and since has served on the International Scientific Committee. She has also served on the Journal of CO_2 Utilization Advisory Board and as an expert in national and international R&I committees. She can be reached at danielle.ballivet-tkatchenko@orange.fr

The Catalyst Review asked Dr. Ballivet-Tkatchenko to share her thoughts on the most pressing needs associated with new catalyst development.

Sustainability goals, circular economy, and net-zero carbon emissions by 2050 are drivers for game-changing technologies in the energy sector and the value chain of chemicals. However, the current options face significant economic and technical hurdles. Nevertheless, thanks to the effects of a shortened learning curve, technologies dealing with renewables, recycling processes, and low-carbon electricity are en route to establishing a new paradigm of a climate-neutral economy. Catalytic technologies remain at the heart of these processes but changing intrinsic basic mechanisms requires new catalysts to be designed and implemented in order to be marketable as early as possible. Prominent catalytic technologies under assessment are:

Carbon-free H_2 Production

Water splitting by electrocatalysis to achieve dihydrogen or green H_2 production is the current technology of choice to replace ongoing carbon-based production. Renewable energy sources have significantly improved the competitiveness of this technology, opening avenues to new hydrogen usage. These sources include chemical energy storage from wind- and solar-powered stations (Power-to-X technologies) and energy carriers for clean mobility (fuel cell). However, the transition toward full deployment of this technology will require a drastic reduction of costs, currently twice those from steam reforming. A significant step forward to achieving a technology breakthrough involves the photoelectrocatalysis of water splitting. Therefore, toxic-free and non-critical (photo)electrocatalysts design is a priority. Moreover, the new candidates need to deliver H_2 on-demand, be flexible enough to cope with fluctuating energy input ideally, and, most importantly, be scalable for small to large scale production.

Carbon-free NH_3 Production

Ammonia, a major global commodity, is mainly produced by the conventional Haber-Bosch process, one of the largest energy-consuming and greenhouse gas-emitting technologies. Deep decarbonization of its production can be achieved by switching to green H_2 feedstock. Besides the well-established chemical markets, ammonia is envisioned as a significant player in the energy sector either as a "drop-in" replacement for fossil fuels or hydrogen carrier/storage. Even carbon-neutral ammonia production under very mild conditions is foreseen thanks to (photo)electrocatalysis technologies. Proof of concept has been demonstrated at the R&D stage, using either H_2 or water as co-feed. For the time being, the design of high-performance catalysts with high faradic efficiency and reaction rate is crucial for the future of the technology, thus enabling decentralized NH_3 production.

Fossil-free Carbon to CO_2 Feedstocks

Biomass feedstock is another game-changer at the forefront of bringing renewable carbon to the fuel and chemicals markets. Generally speaking, transposing the value chain of petroleum suffers from competitiveness. One case study involves biogas production which can be catalytically upgraded either to syngas or methane. Policy incentives for small to medium production scale will ensure a delocalized commercial future for these catalytic technologies.

Is CO_2 the ultimate feedstock for industry? Nature performs well under mild conditions. But the challenges ahead for achieving synthetic photocatalytic conversion of CO_2 into marketable fuels and chemicals are enormous. However, processes involving thermal (photo)electro-, plasma-catalysis technologies with H_2, preferably green, are burgeoning. Moreover, the handful of processes close to market introduction are encouraging signs for CO_2 to enter the fuels and chemicals value chains thanks to decarbonized energy and (photo)electrocatalysis.