U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

Advanced Manufacturing Office

Dynamic Catalyst Science Roundtable

Summary Report

February 26, 2020
Houston, TX

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The U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) Advanced Manufacturing Office (AMO) partners with industry, small business, universities, and other stakeholders to identify and invest in emerging technologies with the potential to create high-quality domestic manufacturing jobs and enhance the global competitiveness of the United States.

This document was prepared as a collaborative effort between DOE AMO, Boston Government Services, and Energetics.

Disclaimer

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1. Executive Summary

The Department of Energy's Advanced Manufacturing Office held an informal roundtable on *Dynamic Catalyst Science (DCS) and Data Analytics* in Houston, Texas, on February 26, 2020. The roundtable brought together leading scientific and technical experts to obtain their insights on the needs for dynamic catalyst science and data analytics to enable a paradigm shift in the approach to catalyst development and chemical manufacturing. The following were the specific key questions addressed: what advanced tools are needed to understand complex industrial catalysts, and what new information can be gained by using temperature, concentration, or pressure transients to perturb the state of a chemical system? The input collected from this event will provide an understanding of the emerging technology landscape for catalysis science that enables a globally competitive chemical manufacturing sector and the real, impactful opportunities for breakthrough research and development (R&D).

This report summarizes the presentations and small group discussions that took place at this event. Note that the results presented here are a snapshot of the viewpoints expressed by the experts who attended the roundtable and may not necessarily reflect those of the broader chemicals industry community.

The first half of the DCS roundtable allowed attendees to share multiple perspectives from recent research results and emerging methods as well as industry needs and considerations. Several common themes emerged during these discussions:

Common Theme #1 – Methods and models are needed to address multi-scale phenomena

A challenging aspect of industrial heterogeneous catalysis is the broad range of length and time scales that must be addressed: An industrial-scale reactor is used to control a molecular-level reaction event. Researchers are considering augmenting physical models with machine learning and multi-scale simulation methods that can utilize structural characterization, microkinetic data, and dynamic and transport phenomena to close knowledge gaps between catalyst formulation, industrial process conditions and global performance. Process industry representatives are interested in coordinated multi-scale models that can utilize information such as molecular-scale surface phenomena to better predict how performance (particularly ways to mitigate catalyst deactivation) may be controlled from the commercial scale.

Common Theme #2 – Dynamic experiments enable the application of machine learning methods

Researchers, catalyst developers and process industry representatives all agreed on the opportunity to employ machine learning to advance the capabilities of DCS. The distinguishing feature of dynamic experiments, whether they utilize temperature, concentration or pressure transients, is the vast amount of data that can be acquired in a short period compared to steady-state methods. With dynamic tools such as this, machine learning can support the development of detailed mechanistic models and kinetic characterization of practical relevance where complex industrial catalysts are studied for reactions in both liquid and gas phases.

Common Theme #3 – Predictive methods are needed that can more rapidly assess catalyst deactivation

Catalytic conversion rates and selectivity undergo significant change over the lifetime of a catalyst. Laboratory tests often show very promising initial performance, which rapidly drops over a short period, before assuming a slower decline at a significantly diminished conversion or selectivity. One catalyst developer in attendance identified catalyst durability as the primary challenge for adopting new catalytic technology in the industry. In addition, methods for accelerating *prediction* of catalyst performance and lifetime without the need for extensive time-on-stream studies was identified as a key focus where efforts should be directed. A common practice is to use accelerated aging, but this can often give rise to phase transformations and new dynamic phenomena that make correlation to long term behavior in the process environment more difficult. There was general agreement on the need to better understand catalyst aging with an emphasis on identifying causes, mechanisms, and rates of deactivation in the early stage of development. To meet this challenge, DCS tools are needed that can collect time-resolved structural data (on the millisecond timescale) that can yield better understanding of transient kinetic information. For catalysts that require frequent regeneration, there are often short-term benefits to regeneration that have negative impacts on the long-term stability. Oxidative regeneration steps may be conducted at high temperatures, so tools should be reliable at $T > 850°C$.

Facilitated discussions during the second half of the DCS roundtable identified several critical knowledge gaps and key R&D needs that could be opportunities for continued advances in catalytic process industries. These are outlined in Table 1-1.

Table 1-1. Summary of Gaps, Opportunities and Collaboration Needs for Development of Dynamic Catalyst Science

Critical Knowledge Gaps	Key Research and Development Opportunities
Multi-Scale Modeling, Simulation, and Data Analytics • Modeling informed by active site changes on different timescales using in situ/operando[1] characterization • Ability to characterize and control the distribution of active sites • Multi-scale integration of kinetics and transport across surface/interfacial and meso, macro scales • Standardized schema and testing protocols – different sources and types of data – no source for consistent parameters among researchers	**Multi-Scale Modeling, Simulation and Data Analytics** • Link kinetic, surface structure and composition characterization through machine learning methods, in addition to physics-based modeling, to develop catalyst assessment methodologies • Better models for integration with dynamic characterization and operando experiments; linking operating environment and materials research • Integration of characterization and process models using data analytics to understand environment-sensitive structure, dynamics and function
Materials • Reproducible catalyst synthesis that can be scaled • Advanced catalyst stabilization methods • Uniform, optimal distribution of sites that can respond to dynamic conditions • Accelerated catalyst deactivation prediction	**Materials** • Catalysts that can handle feedstock flexibility • Catalysts that are robust to changing process conditions • Catalysts that are robust to deactivation
Market and Workforce • Techno-economic information not widely available • Workforce unfamiliar with the process of new catalyst commercialization • Lifecycle analysis could improve the development focus, e.g., CO_2 impacts	**Processes and Reactors** • Integrated development of new catalysts and processes • Sustainable processes that lower CO_2 generation and energy consumption • New reactor design that can implement dynamic catalysis
Collaboration Needs	
Who? Continue to follow U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) models where academia, national labs, and catalyst and chemical manufacturers collaborate to absorb risk at critical decision points. Collaborate through a working group of coordinated computational, modeling and experimental work; develop new tools together.	**What?** • Large data synthesis collaboration • Standardized data collection, analysis, archiving and distribution with defined and reproducible test conditions • Industry-identified toolset needs and feedback • Industry performance goal sharing for directed development projects with scale-up sightline

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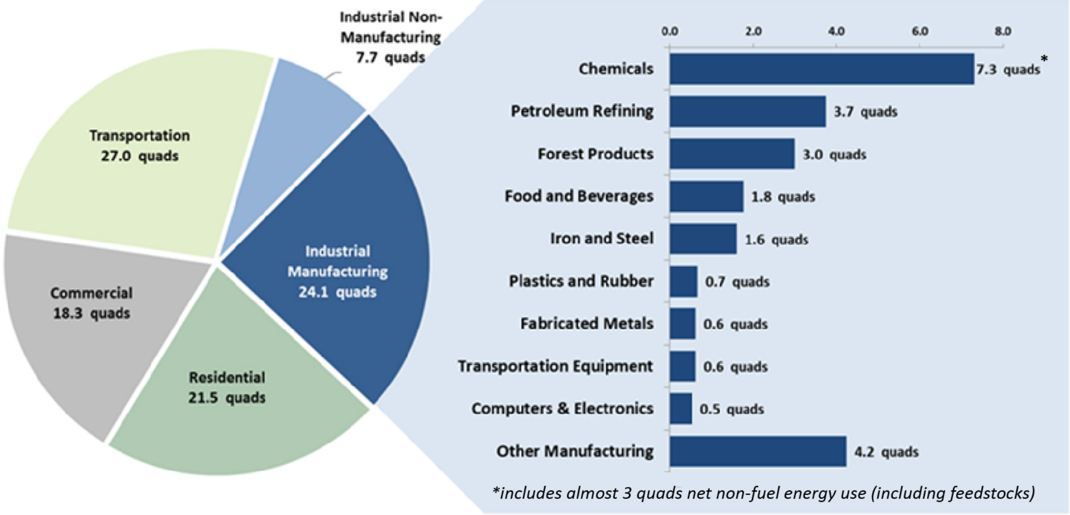
[1] The term operando is generally understood to mean observing the material under actual operating conditions.

2. Background and Roundtable Proceedings

Background

The chemical industry is an important part of the U.S. economy and is the largest exporting sector in the United States, accounting for over 12% of the world's total chemical production making the United States the second-largest chemical-producing nation.[2] The industry is directly responsible for creating more than 500,000 jobs.

The industrial sector is the largest consumer of energy in the United States (Figure 2.1). The U.S. Energy Information Administration (EIA) reports that chemical manufacturing is the largest user among industrial manufacturers (in 2014, EIA adjusted its tabulation of energy feedstock use). Energy is an important component of the costs within the chemical industry and can account for up to 85% of the total production costs for some energy-intensive chemical products.[3] Since 2010, shale gas production in North America has caused a dramatic shift in production costs. Today, the United States is among the lowest-cost producers in the world, attracting record levels of investment in new facilities and expanded production capacity. This shift is also presenting new R&D opportunities that may enable smaller, modular manufacturing.



The industrial sector is the largest consumer of energy in the United States (left figure), with industrial manufacturing accounting for 76% of the sector's energy consumption in 2014. Chemicals manufacturing is the largest consumer of energy of the industrial manufacturers, accounting for 30% of the total (right figure).

Figure 2-1. Overall U.S. Energy Consumption, 2014[4]

Chemical industry R&D is innovative, combining a variety of chemicals, materials, processes and systems to create new technologies and products in high-technology fields with wide industrial applications. Innovation and learning continue to be critical to success and long-term drivers of future economic growth and competitiveness.

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[2] American Chemistry Council, 2019 Guide to the Business of Chemistry.

[3] Ibid.

[4] "Monthly Energy Review," data from U.S. Energy Information Administration, November 2018: Tables 2.1 and 2.4, https://www.eia.gov/totalenergy/data/monthly; "Manufacturing Energy Consumption Survey (MECS): 2014 MECS Survey Data," U.S. Department of Energy, U.S. Energy Information Administration, October 2017: Table 1.2, http://www.eia.gov/consumption/manufacturing/data/2014/. The manufacturing energy consumption shown here reflects energy used for all purposes, including almost 3 quads of net non-fuel energy use in chemicals manufacturing.

Manufacturing remains the essential core of the U.S. innovation infrastructure and is critical to economic growth and national defense. Experts point to a gap in the innovation continuum that exists between R&D activities and the deployment of technological innovations in the domestic production of goods. Concerns have been raised that this gap could have long-term negative consequences for the economy and the defense industrial base. As global competition to manufacture advanced products intensifies, the performance of the country's innovation ecosystems must improve. Industry, academia and government partners need to leverage existing resources, collaborate and co-invest to nurture manufacturing innovation and accelerate commercialization.

Roundtable Overview

The Advanced Manufacturing Office (AMO) within DOE's EERE partners with private and public stakeholders to improve U.S. competitiveness, save energy, create high-quality domestic manufacturing jobs, and ensure global leadership in advanced manufacturing and clean energy technologies. AMO invests in cost-shared research, development and demonstration of innovative, next-generation manufacturing processes and production technologies that will improve efficiency and reduce emissions, reduce industrial waste and reduce the lifecycle energy consumption of manufactured products. The results of this investment include having manufacturing energy efficiency harnessed as a competitive advantage and cutting-edge clean energy products competitively manufactured in the United States. AMO is particularly interested in the challenges associated with advanced manufacturing technology related to the energy-intensive chemical industry.

Dynamic Catalyst Science:

Advanced tools that use temperature, concentration, or pressure gradients to perturb the state of a chemical system to advance our understanding of complex industrial catalysts, thereby enabling a paradigm shift in catalyst science.

The roundtable on *Dynamic Catalyst Science (DCS) and Data Analytics* was held on February 26, 2020, to collect chemical industry stakeholders' perspectives on future research priorities. Representatives from the chemical industry, DOE national laboratories and academia gathered in Houston, Texas, to hear expert speakers and participate in facilitated discussions regarding technology needs and opportunities for dynamic catalyst science and data analytics. The following were the specific key questions addressed: what advanced tools are needed to understand complex industrial catalysts, and what new information can be gained by using temperature, concentration, or pressure transients to perturb the state of a chemical system? Discussion topics focused on critical knowledge gaps, key research and development opportunities, and workforce and collaboration needs. The agenda for the roundtable can be found in Appendix A, and Appendix B provides the full list of attendees. The acronyms used in this report are defined in Appendix C.

Figure 2-2. DCS and Data Analytics Roundtable Facilitated Session

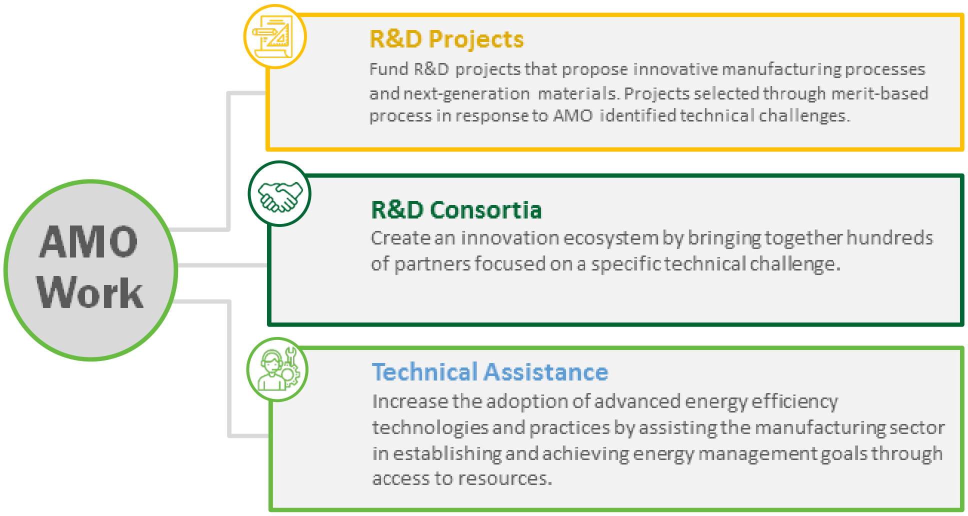
Figure 2-3. Roundtable Group Photo (facilitated sessions in insets)

3. The Advanced Manufacturing Office's Interest in Chemical Manufacturing and Catalysis

An overview of DOE AMO interest in the chemical industry and catalysis was provided by Dr. G. Jeremy Leong, Technology Manager, R&D Projects. Technology innovation through applied R&D in advanced manufacturing and energy is a foundation for economic growth and jobs in the United States. The mission of AMO is to catalyze R&D and adoption of energy efficient advanced manufacturing technologies and practices to drive U.S. economic competitiveness and energy productivity. As part of its mission, AMO supports a range of projects addressing chemical industry energy challenges, through a three-pronged approach (see Figure 3-1, below).

Significant growth in production volume is expected within the chemical sector. Since 80% - 90% of all chemical manufacturing relies on catalysts; any improvements to catalyst selectivity and reaction conversion could potentially have great impact on energy use. For the chemicals that require the most energy to manufacture, it is estimated that new catalysts and related process improvements could reduce the energy intensity of these products by 20% to 40% by 2050[5]. The need for improved catalyst performance is requiring interdisciplinary approaches for catalyst design through computational technologies, enabling more directed experimentation and validation.

Today, manufacturing processes are centralized, large-scale and designed for steady-state. Manufacturing processes in the future could be distributed, smaller scale, robust and flexible to changing operational conditions that may be driven by variable or intermittent renewable energy. Despite the flexible conditions, production still needs to be energy efficient and cost-effective. In order to facilitate this drastic change in manufacturing, advanced tools are needed to understand industrial catalysts, which tend to be complex, multicomponent systems with ill-defined or amorphous surfaces. Current analysis tools can only provide global kinetic information.



Fund R&D projects that propose innovative manufacturing processes and next-generation materials. Projects selected through merit-based process in response to AMO identified technical challenges.

Create an innovation ecosystem by bringing together hundreds of partners focused on a specific technical challenge.

Increase the adoption of advanced energy efficiency technologies and practices by assisting the manufacturing sector in establishing and achieving energy management goals through access to resources.

Figure 3-1. Three Pillars of the AMO Program

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[5] Technology Roadmap: Energy and GHG Reductions in the Chemical Industry via Catalytic Processes, International Energy Agency, 2013, https://www.iea.org/publications/freepublications/publication/TechnologyRoadmapEnergyandGHGReductionsintheChemicalIndustryviaCatalyticProcesses.pdf

To address the challenges and opportunities outlined above, the Chemical R&D Projects portfolio research efforts are grouped into one of three main focus areas:

1.) **Catalyst Science and Design –** focuses on developing tools to understand catalytic mechanisms in order to improve existing and design new catalysts that will produce technical advances in chemical conversion technology and benefits in energy efficiency in specific applications.
2.) **Intensified Processes –** focuses on combining reactions and separations or developing modular processes, including electrochemical processes, targeted at reducing the energy intensity of the chemical industry. Modularized processes also enable flexibility at small to medium scales, while electrochemical processes provide high selectivity, control of reaction kinetics and fewer emissions.
3.) **Enabling Technologies –** focuses on developing technologies that permit researchers to incorporate innovative tools or capabilities within their work at all levels to accelerate process development cycles. Technologies include modeling and simulation, characterization technologies, and machine learning and data analytic techniques.

Dr. Leong concluded his presentation by stating that the purpose of the 2020 DCS roundtable was to identify the critical knowledge gaps in catalyst science that could enable more flexible chemical manufacturing in the future, with special emphasis on employing advanced tools to understand complex industrial catalysts by learning from the chemical response to temperature, concentration or pressure transients.

4. Catalytic Research and Process Industry Perspectives

Research Capabilities and Existing Efforts

Dr. Lars Grabow welcomed participants to the University of Houston, a Hispanic-serving institution with one of the most diverse student bodies among research-intensive universities. Founded in 1952, the program annually produces 80–90 graduates with Bachelor of Science degrees and ca. 20 graduates with PhD degrees in chemical engineering. The department's current funding level is approximately $450,000/FTE/year, supporting its key research competencies in catalysis and reaction engineering; nanoporous, electronic and polymeric materials; and biomolecular engineering.

There were five morning presentations in the roundtable meeting; these were intended to capture industry perspective and existing capabilities in dynamic catalysis science. Mr. David West from SABIC kicked off this perspective with a candid reminder of the history of industrial chemical commercialization and the evolution of catalyst discovery. Mr. West ended with an open-ended reflection on the relationship between innovation, the marketplace, and the Edisonian[6] approach.

Dr. Lars Grabow and Dr. A.J. Medford provided an academic perspective on the challenges, needs and efforts under way at the University of Houston and Georgia Institute of Technology, respectively. Dr. Grabow emphasized the importance of understanding the reaction mechanism through DCS and the need for more detailed mechanistic knowledge and models with practical relevance that provide convergence of length scales. Dr. Medford talked about the use of data science in DCS and how machine learning may or may not extract meaning out of the large dynamic data sets. He pointed out that combining machine learning with physics and chemistry is essential to understanding what is known and what is not known.

The DOE National Laboratories are key contributors to the existing R&D in dynamic catalysis. Dr. Rebecca Fushimi from Idaho National Laboratory discussed recent activities using the temporal analysis of products (TAP) pulse response methodology to understand catalysts for oxidative coupling of methane. Dr. Fushimi discussed the benefits of combining TAP with more advanced spectroscopic characterization in a "spectrokinetic" reactor that could directly address the materials structure/activity knowledge gaps.

Finally, Dr. Jeff Weissman from Precision Combustion, Inc., concluded the morning presentations by talking about innovative designs for catalyst application and development. This small, private business has used Small Business Innovation Research (SBIR) awards to better understand catalyst durability, lifetime, and performance and to learn more about identifying, protecting, and enhancing catalytically active sites.

Catalytic Process Industry Perspectives

The afternoon session for the roundtable had no formal presentations; rather, it was designed to facilitate conversation around process industry perspectives. In this session, process industry stakeholders in attendance took turns sharing their perspectives on the needs and considerations for DCS to accelerate catalyst development and enable efficient chemical manufacturing. Attendees joined in an open discussion in response to each participant. The industry perspectives and subsequent discussion are summarized below by topic area. The summaries should not be read as consensus opinion but rather as a merging of ideas and opinions into a more readable form. Appendix D contains a list of individual industry comments by topic area captured during the afternoon session.

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[6] Loosely explained as discovery by trial and error rather than a systematic theoretical approach. The suggestion was to try a lot of things, having multiple Edisonian systems, rather than trying a lot of diverse things.

Catalyst Chemistry versus Catalyst Lifetime

Industrial researchers noted that knowledge gaps exist between fundamental and applied research where, in practice, applied industrial research requires more fundamental understanding, and fundamental science requires more insight from the end use. When considering dynamic catalyst science or, more broadly, catalysis, major considerations include catalyst lifetime, performance and scale-up. Evaluating the initial catalyst deactivation rates and overall catalyst lifetime may be inversely coupled. Understanding the phenomena that drive catalyst aging by developing structure-linked kinetic models that capture evolution of activity across short and long timescales, in addition to the conventional characterization of fresh or green catalysts, would be helpful. Researchers should consider employing and coupling a wide variety of toolsets to gather information on catalyst lifetime. For example, leveraging data analytics and machine learning coupled with transient characterization techniques such as TAP or frequency response methods could provide insight on catalyst deactivation at early stages.

Importance of Catalyst Data Quality and Performance Metrics

Many industry attendees noted that vast amounts of catalytic data exist in the literature that could be amenable to machine learning, but data cleanliness and consistency are constant challenges in this space. Since dynamic experiments are highly amenable to machine learning, the DCS toolbox could become a learning platform that can extract critical information, such as surface reaction phenomena, to potentially inform and provide actionable insight toward the catalyst development/design cycle. To accomplish impactful progress in this space, the roundtable attendees identified the needs for standard catalyst performance metrics and for a way to acquire, analyze and organize data; to ensure quality and interpretability precision and reproducibility; and to build shared, robust and reliable content over time.

Integrating Catalyst and Process Development

From an industrial perspective, a holistic view of developing new and optimizing existing processes is essential, given the multiple layers associated with scale-up at both the catalyst and reactor levels. For industry, it is important to consider co-optimizing or co-designing the catalyst and reactor system including a focus on the reactor products, activity change during time on stream, and regeneration requirements, as opposed to solely on catalyst selection and respective yields. This can be accomplished only through multi-scale development processes that consider the full atomic-to-reactor scale based on intrinsic physicochemical behaviors. However, better kinetic models, e.g., that offer microkinetic data, on industrial catalysts are needed to replace lumped models that do not discriminate mechanistic detail. This is especially true when it comes to novel, alternative reaction pathways and reactor designs. Some attendees identified a need for a step change improvement to de-risk new technologies since the chemical industry tends to be risk-averse. From historical precedents, industry has a higher likelihood of pursuing investment in incremental improvements to known inventions with demonstrated utility, especially when considering the risks as well as the weighted average cost of capital (WACC). In addition, considering the back-end innovations beyond catalyst improvements at the system level is key to targeting technological advancements toward increased efficiency.

Possible Enabling Role of DCS in Sustainability

Industry is interested in sustainability and environmental impact applications, including technologies to reduce/reuse/capture emissions, reduce hazardous waste and produce value-added chemicals from biofeedstocks. Modularized technologies present the opportunity to spread/dilute the risk by potentially decreasing costs through standardization with no variation in performance. Modularized technologies also have lower mass and thermal inertia and are naturally suited to be more responsive to forced dynamic operation. Less expensive, more available sources of electricity could increase the viability and use of electrochemical methods. Given the emerging nature of many modularized technologies that employ electrochemical, photochemical, or other lower thermal budget as well as hybrid approaches, there are prime opportunities for leveraging DCS to gain a better understanding of the mechanisms by which these technologies convert energy and feedstock/reactants to chemicals. Industry participants stressed that distributed manufacturing through modular approaches is different from manufacturing in large complexes because economies of scale-up can potentially be addressed by economies of scale-out. Multiple industry attendees mentioned the development and use of small modular units as a potential future route for the chemical manufacturing industry.

Role for Public–Private Partnerships in De-Risking DCS

There was particular emphasis on the need for an industry-informed, concerted, facilitated and collaborative programmatic effort to build an inter- and multi-disciplinary team to identify, evaluate, manage and utilize catalyst performance data. Multiple attendees noted that a comprehensive framework effort is too large for a single entity to take on and noted the consortium model as a way to address this challenge while allowing for a balance between data sharing and intellectual property preservation. From an industry perspective, most companies will not be convinced that a single entity could successfully develop new DCS tools, and thus a consortium approach is needed. New DCS tools would be required not only to show sufficient improvements at a technology level but also to demonstrate utility by multiple groups or a consortium. Demonstrating and validating DCS and DCS tools is necessary to de-risk industry investment. Roles for federal government would include funding of consortia and also funding DCS over the long term to develop and demonstrate the technology.

Common Themes

The first half of the DCS roundtable provided an opportunity to share multiple perspectives, from existing data science and research to industry needs and considerations. The three common themes that emerged in the morning presentations and discussions are summarized below.

Common Theme #1 – Methods and models are needed to address multi-scale phenomena

A challenging aspect of industrial heterogeneous catalysis is the broad range of length and time scales that must be addressed: An industrial-scale reactor is used to control a molecular-level reaction event. Researchers are considering augmenting physical models with machine learning and multi-scale simulation methods that can utilize structural characterization, microkinetic data, and dynamic and transport phenomena to close knowledge gaps between catalyst formulation, industrial process conditions and global performance. Process industry representatives are interested in coordinated multi-scale models that can utilize information such as molecular-scale surface phenomena to better predict how performance (particularly ways to mitigate catalyst deactivation) may be controlled from the commercial scale.

Common Theme #2 – Dynamic experiments enable the application of machine learning methods

Researchers, catalyst developers and process industry representatives all agreed on the opportunity to employ machine learning to advance the capabilities of DCS. The distinguishing feature of dynamic experiments, whether they utilize temperature, concentration or pressure transients, is the vast amount of data that can be acquired in a short period compared to steady-state methods. With dynamic tools such as this, machine learning can support the development of detailed mechanistic models and kinetic characterization of practical relevance where complex industrial catalysts are studied for reactions in both liquid and gas phases.

Common Theme #3 – Predictive methods are needed that can more rapidly assess catalyst deactivation

Catalytic conversion rates and selectivity undergo significant change over the lifetime of a catalyst. Laboratory tests often show very promising initial performance, which rapidly drops over a short period, before assuming a slower decline at a significantly diminished conversion or selectivity. One catalyst developer in attendance identified catalyst durability as the primary challenge for adopting new catalytic technology in the industry. In addition, methods for accelerating *prediction* of catalyst performance and lifetime without the need for extensive time-on-stream studies was identified as a key focus where efforts should be directed. A common practice is to use accelerated aging, but this can often give rise to phase transformations and new dynamic phenomena that make correlation to long term behavior in the process environment more difficult. There was general agreement on the need to better understand catalyst aging with an emphasis on identifying causes, mechanisms and rates of deactivation in the early stage of development. To meet this challenge, DCS tools are needed that can collect time-resolved structural data (on the millisecond timescale) that can yield better understanding of transient kinetic information. For catalysts that require frequent regeneration, there are often short-term benefits to regeneration that have negative impacts on the long-term stability. Oxidative regeneration steps may be conducted at high temperatures, so tools should be reliable at T > 850°C.

5. Knowledge Gaps, Research Opportunities and Possible Collaboration Roles to Accelerate Dynamic Catalyst Science

The final session of the DCS roundtable comprised a facilitated discussion using a storyboarding approach. A facilitator guided this discussion by first setting some ground rules and then posing questions to participants. Individuals were asked to complete idea cards that were collected and grouped at the front of the room. All attendees were equally encouraged to share their ideas on knowledge gaps, research opportunities, and possible roles for collaboration to accelerate catalyst development and enable efficient chemical manufacturing. The three moderated questions are outlined in the text box on the right. Detailed results from this facilitated discussion can be found in Appendix E; the findings are summarized below.

Moderated Questions

- What are the critical knowledge gaps in catalyst science needed to advance chemical manufacturing at present?
- What are the key research opportunities in catalyst science that can impact productivity in chemical manufacturing in the future?
- What are the roles of industry, academia and government in the development of new tools?

Knowledge Gaps or Limitations

Roundtable attendees identified a range of areas where the critical knowledge gaps or limitations exist in accelerating catalyst development and enabling efficiency in chemical manufacturing using DCS and data analytics. While some ideas were similar, building on the comments of others, other ideas were distinct. It was interesting to note that the ideas brought forth spanned from fundamental analysis to workforce and demonstration—a testament to the breadth of attendees and their comprehensive perspective. Knowledge gaps were grouped into the following categories:

- Mechanistic knowledge, including modeling, simulation and data analytics
- Characterization and tools
- Controlled and reproducible materials synthesis
- Reaction conditions (particularly, dynamic)
- Testing and demonstration
- Scale-up
- Market, workforce and training

Mechanistic knowledge and characterization – A lack of standardized data sets and testing protocols was identified as a hindrance for comparing research results. Conventional methodologies that characterize materials at static or steady-state conditions were called out as a limit in the ability to apply machine learning methods to find new correlations. The development of multi-scale materials models reflecting active site changes under dynamic operation, as well as their integration with microkinetics and computational fluid dynamics to describe reaction and transport kinetics, was another analytical limitation. In a related set of ideas, attendees identified operando characterization of dynamically formed active sites as a significant knowledge gap in catalyst science.

Materials – The ability to predict catalyst stability/lifetime and to design reproducible catalysts with optimal distribution of active sites were some of the materials gaps that were identified. Working with complex industrial materials and complex kinetics was another gap. There is a gap in understanding how to control catalyst synthesis for reproducible performance.

The complete list of identified knowledge gaps, including gaps in technology scale-up, techno-market, workforce, and reaction conditions can be found in Appendix E-1.

Research Opportunities

Considering the knowledge gaps that were identified during the first moderated question, attendees were prompted to address those limitations with recommended and necessary research opportunities. Unsurprisingly, the research ideas put forth by attendees fell into similar categories. Research opportunity ideas were grouped into the following categories:

- Mechanistic knowledge, including modeling, simulation and data analytics
- Characterization and tools
- Materials
- Processes
- Reactor design
- Deployment and scaling

After the research ideas were collected and grouped at the front of the room, attendees were asked to vote on what they individually felt were the R&D priorities. Figure 5-1 is a collection of key phrases from the priority research opportunities identified by the group. Research opportunities receiving the most votes are shown in blue and green. Detailed results can be found in Appendix E-2.

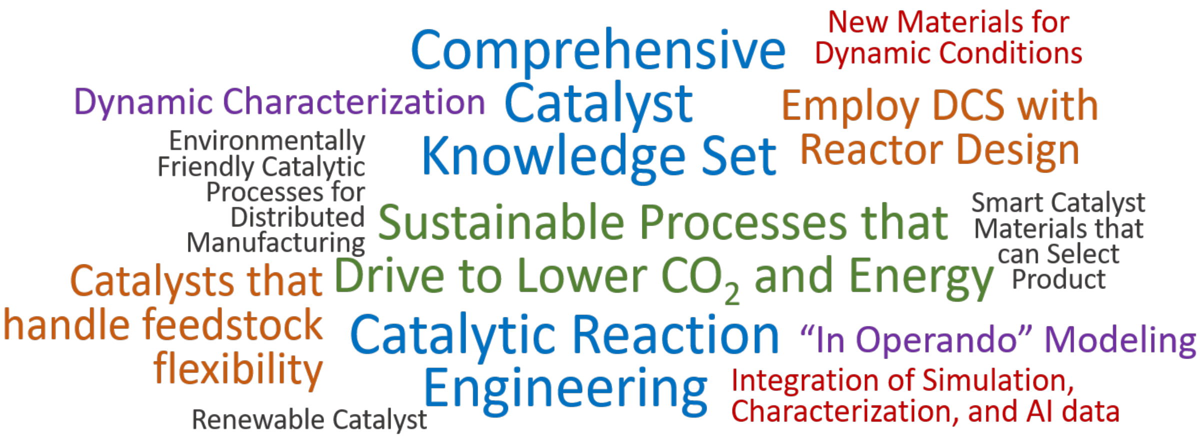

Figure 5-1. Priority Research Opportunities

The three highest-scoring research needs are explained here. Note that Priorities 1 and 2 received the same number of votes (eight), while Priority 3 received two fewer votes (six).

Priority 1: Comprehensive Catalyst Knowledge Set – Attendees identified the need to link well-defined kinetics, surface structure, operation conditions, catalyst composition and reaction parameters together with machine learning to develop a comprehensive catalyst knowledge set.

Priority 2: Catalytic Reaction Engineering – Attendees prioritized the need for renewed investment in catalytic reaction engineering to develop catalyst and reactors in tandem as well as multi-scale reactor models that can take phenomena into account that vary widely across time and length scales.

Priority 3: Sustainable Processes that Drive to Lower CO_2 Generation and Energy Consumption – Sustainability was a topic that arose throughout the roundtable. Attendees prioritized the need for sustainable processes that lower CO_2 generation and energy consumption. Some examples provided include dilute CO_2 separations, catalysis for CO_2 conversion to low-energy fuels and chemicals, electrocatalytic pathways for CO_2

conversion, energy efficiency in manufacturing, reuse of emissions, and catalysis for ambient CO_2 conversion and removal.

Roles and Collaboration

The third moderated question was considered in parallel with the first two questions. When attendees brainstormed the first two moderated questions, they were encouraged also to write down their associated ideas for roles and collaboration. Roles were loosely defined to include industry, academia and government.

Collaboration between industry, academia and government was identified as necessary for pre-competitive research, large data synthesis, and standardized data collection, archiving, and distribution. There was a suggestion that a research hub would encourage teaming between academia, national labs, and catalyst and chemical manufacturers. A research hub could be used to provide access to unique resources that are essential to DCS, such as the TAP reactor system and other specialized instrumentation, in a “user facility”-type arrangement. The facility could also provide integration of these instruments with HPC capabilities and multi-scale modeling. Collaboration would help to absorb risk at critical decision points.

Attendees suggested that it would be helpful for industry to share performance goals for directed development projects and to define the toolsets needed, with feedback (good and bad).

6. Conclusion

The roundtable concluded with Dr. Jeremy Leong thanking the University of Houston for hosting the meeting. Attendees were informed that the presentations would be available on the DOE AMO website and that this roundtable report would be published a few months after that.

APPENDIX A: AGENDA

Dynamic Catalyst Science Roundtable

Initiated by the DOE/EERE Advanced Manufacturing Office

University of Houston
Student Center South | Heights Room 224 | 4455 University Drive
Houston TX | 10 AM – 4:15 PM, February 26, 2020

Time	Activity
9:30 AM – 10:00 AM	Check in and Networking
10:00 AM – 10:20 AM	Welcome, EERE AMO – Introduction and Objectives • Meeting Hosts: Lars Grabow and Mike Harold, University of Houston • Jeremy Leong, Technology Manager, Advanced Manufacturing Office
10:20 AM – 10:40 AM	Industry Perspective, R&D Challenges, Opportunities • David West, SABIC
10:40 AM – 11:00 AM	Connecting Atomistic Modeling, Laboratory and Industrial Scales • Lars Grabow, University of Houston
11:00 AM – 11:20 AM	Structure/Kinetics of Complex, Industrial Catalysts • Rebecca Fushimi, Idaho National Laboratory
11:20 AM – 11:40 AM	Extracting Knowledge for Industrial Catalysis through Machine Learning • A.J. Medford, Georgia Institute of Technology
11:40 AM – 12:00 AM	Industry Perspective, R&D Challenges, Opportunities • Jeff Weissman, Precision Combustion, Inc.
12:00 PM – 1:00 PM	Light Lunch and Refreshments (Provided by University of Houston)
1:00 PM – 2:30 PM	Chemical Manufacturing Industry Stakeholder Research Priorities *Facilitated Discussion,* Sabine Brueske, Energetics • **Chemical Manufacturing Representatives,** To start the discussion, industry representatives are invited to share a short overview of their perspective on the R&D needs for dynamic catalyst science to accelerate catalyst development and enable efficient chemical manufacturing.
2:30 PM – 2:45 PM	Break

Time	Activity
2:45 PM – 3:45 PM	**R&D Gaps and Opportunities** *Facilitated Discussion Topics* • What are the critical knowledge gaps in catalyst science needed to advance chemical manufacturing at present? ▪ What are the most impactful tools that are being used now, their advantages and limitations? ▪ What advanced capabilities are essential for the future, e.g. high-performance computing (HPC), data analytics, structural/kinetic characterization *in operando*, multi-scale modeling/simulation? ▪ What opportunities can be uniquely addressed using dynamic catalyst science? ▪ What are the current limitations in the integration of catalyst science, reaction engineering and process development? • What are the key research opportunities in catalyst science that can impact productivity in chemical manufacturing in the future? ▪ What are the driving forces for energy efficiency in chemical manufacturing? How can advanced catalyst help meet these goals? ▪ What chemical manufacturing opportunities (e.g. feedstocks, products, processes) are on the horizon for the next 5, 20 years and what catalysis R&D is needed to realize these opportunities? ▪ To what extent will chemical manufacturing shift to distributed processes and how will advanced catalysts be needed? • What is the role of industry, academia and government in the development of new tools? ▪ Are there research themes and topics that industry prefers to pursue collaboratively versus internally? ▪ What are the current impediments to collaboration across industry, academia and government and how can they be addressed?
3:45 PM – 4:00 PM	**General Consensus of Top R&D Priorities** *Facilitated Discussion*
4:00 PM – 4:15 PM	**Next Steps and Adjourn** • Jeremy Leong, Technology Manager, Advanced Manufacturing Office

Appendix B. List of Roundtable Participants

Name	Organization
Sabine Brueske	Energetics (facilitator)
Peter Ciesielski	National Renewable Energy Laboratory
Rebecca Fushimi	Idaho National Laboratory
Lars Grabow	University of Houston
Javier Guzman	ExxonMobil
Wenyu Huang	Ames Laboratory
Barbara Kimmich	LyondellBasell
Ted Krause	Argonne National Laboratory
Dheeraj Kumar	Celanese
Jeremy Leong	Advanced Manufacturing Office
Andrew Medford	Georgia Institute of Technology
Carl Mesters	Shell
Theresa Miller	Energetics
Staci Moulton	ForgeNano
Ignasi Palou-Rivera	Rapid Advancement in Process Intensification Deployment (RAPID) Institute
Jim Parks	Oak Ridge National Laboratory
Cory Phillips	Conoco-Phillips 66
John Sofranko	EcoCatalytic
Robert Weber	Pacific Northwest National Laboratory
Jeff Weissman	Precision Combustion, Inc.
David West	SABIC
Brandon Wood	Lawrence Livermore National Laboratory

Appendix C. List of Acronyms

Acronym	Definition
AI	Artificial Intelligence
AMO	Advanced Manufacturing Office
CO_2	Carbon dioxide
DCS	Dynamic catalyst science
DFT	Density functional theory
DOE	U.S. Department of Energy
EERE	Office of Energy Efficiency and Renewable Energy
GHG	Greenhouse gas
INL	Idaho National Laboratory
IP	Intellectual property
LCA	Lifecycle analysis
NDA	Non-disclosure agreement
pv	Photovoltaic
R&D	Research and development
RD&D	Research, development and demonstration
TAP	Temporal analysis of products
VTO	Vehicle Technologies Office
WACC	Weighted average cost of capital

Appendix D. Process Industry Comments and Perspectives

Catalyst Chemistry and Catalyst Lifetime
There is a disconnect between industrial research and applied/fundamental science. We need to make the connection between transient behavior in catalysis and actual behavior in a refinery or chemical plant.
Looking at the initial catalyst selectivity and looking at catalyst longevity may be inversely coupled. One is easy to study, one is hard.
Consider gathering information on catalyst lifetime from machine learning, including understanding early activation of catalysts using TAP. Because it is transient, is it possible to pull out the deactivation information early and characterize it in the early stage?
It would be helpful to understand the correlations with aging catalysts. Consider developing kinetics models around aged catalysts rather than green catalysts.
Raw materials can impact testing and scale up. It is one of the causes of variability in catalyst science.
If a company provided a specification sheet on the needs for a catalyst coating, that would allow for the design of a new material. The specifications would need to include the desired catalyst lifetime as that determines the testing approach.
Importance of Catalyst Data Quality and Performance Metrics
There is a vast amount of data on catalyst selectivity, activity, and stability that is amenable to machine learning.
Dynamic catalyst science is a toolbox. If you run experiments the right way that are amenable to machine learning, it becomes a learning toolkit.
We can use machine learning to extract information such as surface phenomena.
The industry needs standards/metrics for catalyst performance and a way to organize the data to ensure data quality and to build shared content over time. For example, we could have a standard for TAP reactors and run a campaign for data, then conduct quality control at multiple industry labs to test and assure accuracy.
We need to organize the collection of catalysis performance data, including a facilitated program to integrate it all, and the right people and skills to manage identification and utilization of the data.
The economics of capital equipment still is an open question for DCS. The industry can shave costs, but it needs precise performance without variability.
Catalysts as Part of Reactor and Process Design
There are lots of layers in process scale up, at both the catalyst level and reactor level. The industry needs a step change improvement to de-risk new technology. Without a step change in improvement, the chemical industry will likely not invest since it is extremely risk adverse.
Researchers need to take a holistic view of optimizing processes when considering DCS – we need the best catalyst for the process, not the best process for the catalyst.
We need a multi-scale development pathway that lets us see how to get from atomic to commercial scale.
The chemical industry focuses on incremental opportunities with known inventions that have been proven already. New technology has to be different, but there needs to be small steps in order for the industry to check viability.
The weighted average cost of capital (WACC) is the most important factor influencing investment decisions. Industry is seeking small incremental opportunities for improvement.
Focusing on process efficiency is more important than focusing on catalyst development and improvement alone.

The focus should be on the product from the reactor, not just the catalyst selection and yield. Industry research should look at back end innovations beyond catalysts, for example, improvement in chemical separations.
There needs to be sufficient improvement in a plant's product yield for a company to invest in DCS technologies. A 5% improvement in product yield has a lot of risk associated with it; improvement in product yield would need to be higher than that for industry investment.
We need to know what the engineered structure of the catalyst/reactor looks like and then borrow scaling best practices from other industries.
The upfront catalyst research cost is a tiny part of the overall cost of a project.
Is the goal of DCS to replace current catalytic processes, or to drop in an improved catalyst in current processes? A drop-in catalyst is different than greenfield (developing a completely new process).
Possible Enabling role of DCS in Sustainability
Sustainability is of interest to the industry, including technologies to reduce/reuse/capture emissions, reuse hazardous waste, and value-added chemicals from captured CO_2.
Other sustainability and environmental impact applications may include chemicals from biofeedstocks and chemical production via electrochemistry that is enabled by cheap electricity from renewable sources.
Understanding the activation of zeolites may be quicker with a TAP system.
It is important to consider rates and yields in a given application, but researchers also need to consider heat management.
New catalysts for small scale remote CO_2 capture may be of interest to the industry.
Consider using TAP to develop catalysts for plastics and renewables.
Distributed manufacturing is different than large manufacturing complexes; the objectives are different, and the catalyst role is different.
We are in an era where small modular units may work. They spread out the risk by shaving cost through standardization while forgoing variation in performance. It was noted by a few that it becomes too costly to operate modular units at high temperature (above about 900°C).
Safety is near and dear when working with hazardous chemicals. The industry should also focus on safety issues when discussing catalyst applications.
Role for Public-Private Partnerships in De-Risking DCS
No one wants to be first to demonstrate a new technology. The industry would rather partner with an entity or organization that wants to try a new technology. There is possibly a role for DOE to work with small scale companies to demonstrate new technologies.
To convince a company that a new technology is worthwhile and the data is real, we need more than just money. We need groups or consortia to show it is real.
DCS commercialization is too big for one company to take on, we should consider multiple sites.
Government can help by funding consortia, for example, a center where researchers could do experiments with TAP reactors. Industry can run hot or cold when funding new technologies, but government can maintain the funding focus.
Are there structural things DOE can do to help with intellectual property (IP) for DCS? Perhaps DOE can develop models to handle IP more effectively.
Intellectual property rights are a big issue.
Is DOE doing any research to identify precious metal alternatives that may be valuable to the catalysis industry?

Appendix E. Summary of Facilitated Results

TABLE E-1. CRITICAL KNOWLEDGE GAPS OR LIMITATIONS

What are the Critical Knowledge Gaps, or Limitations in Dynamic Catalysis Science?						
Mechanistic Knowledge, including Modeling, Simulation and Data Analytics	**Characterization and Tools**	**Materials**	**Reaction Conditions**	**Scale Up**	**Testing and Demonstration**	**Market/Workforce /Training**
Multi-scale modeling and simulation informed by active site changes on different time scales • Multi-scale integration of surface interfacial and meso, macroscales in catalyst and reactor models	In-situ/operando characterization of dynamically formed active sites	Making catalyst with uniform active sites under dynamic conditions	Catalysis in condensed phase. This is needed to enable current and future trends towards sustainability, feedstock flexibility and electrocatalysis	Being able to translate dynamic observations to reaction kinetics	Which type of reactions or materials can benefit from dynamic operation?	Techno-market information not available
Definition of what data is needed to enable valuable Machine Learning to advance catalysis	Understanding how to characterize and control the distribution of transient active sites	Making catalyst with optimal distribution of sites		Translation from transient data to activity, selectivity and stability with validation at the scale of the reactor		Workforce – lack of understanding of what it takes to commercialize a new catalytic process

What are the Critical Knowledge Gaps, or Limitations in Dynamic Catalysis Science?

Mechanistic Knowledge, including Modeling, Simulation and Data Analytics	Characterization and Tools	Materials	Reaction Conditions	Scale Up	Testing and Demonstration	Market/Workforce /Training
There is no standardized schema and dynamic testing protocol	Structural/kinetic characterization of in-operando at relevant timescales (e.g. millisecond time resolution)	Better ways to make reproducible catalysts that can be scaled up		Understanding how dynamic catalyst behaviors impact industrial scale performance (predictive tool)		For sustainable processes we need life cycle analysis (LCA) to drive working on the right new technologies; including CO_2 footprint
Modeling – combing microkinetics with computational fluid dynamics and process modeling	In-operando testing capability under near commercial conditions	Complex materials (surface/bulk) and complex kinetics		Connecting short and long timescales in catalyst performance		
The sources and types of data are different	Knowing how reactive sites relates to side reactions	Durability predictions under dynamic conditions (non-steady state)		Understanding the process and working backwards to develop the catalyst		

What are the Critical Knowledge Gaps, or Limitations in Dynamic Catalysis Science?						
Mechanistic Knowledge, including Modeling, Simulation and Data Analytics	**Characterization and Tools**	**Materials**	**Reaction Conditions**	**Scale Up**	**Testing and Demonstration**	**Market/Workforce /Training**
Lack of accessible database for consistent kinetics and parameters for key catalytic reaction steps. Sources: DFT and TAP				Lack of economics in scaling down and scaling out		
Taking advantage or mitigate dynamic behavior control points						

TABLE E-2. KEY RESEARCH OPPORTUNITIES

What are the Key Research Opportunities in Catalyst Science that Can Impact Productivity?					
Mechanistic Knowledge, including Modeling, Simulation and Data Analytics	**Characterization and Tools**	**Materials**	**Processes**	**Reactor Design**	**Deployment and Scaling**
**** (4) Research towards “in operando” modeling: heterogeneity in materials and dynamic operating environments (environment and material research)	******** (8) Link microkinetics (e.g. TAP), surface structure and composition characteristics (e.g. using microscopy/operando/ x-rays/neutrons) together with machine learning to develop comprehensive catalyst knowledge set	****** (6) Catalysts that can handle feedstock flexibility	******** (8) Need renewed investment in catalytic reaction engineering – impact of transport on reaction in affecting space-time yield and selectivity	****** (6) Reactor design for dynamic catalyst – hybrid for change	**(2) Need environmental friendly catalytic processes for chemical manufacturing shift to distributed process
*** (3) In the catalyst environment we need to understand environment-sensitive structure, dynamics and function through integration of simulation and characterization with AI/data analytics. Multi-lab/industry/academia teams. • e.g., couple higher order catalyst architecture to atomistic dynamic phenomena	**** (4) Dynamic characterization. Better “operando” (higher time resolution), structure and microkinetics through new tools	*** (3) New materials designed for dynamic conditions with optimized techno-market performance	******* (7) Sustainable processes that drive to lower CO_2 and energy in processes, relating to CO_2 utilization • Low CO_2 separations; materials, life cycle analysis • Catalysis for low energy fuels and chemicals • Research into energy efficiency in manufacturing and renewables • Research reuse of emissions • Catalysis for ambient CO_2 conversion and removal	Less severe high efficiency dynamic electrocatalytic reactors that are modular and multi-phase	** (2) Renewable catalyst: solar pv, solar thermal, distributed cyclic

What are the Key Research Opportunities in Catalyst Science that Can Impact Productivity?

Mechanistic Knowledge, including Modeling, Simulation and Data Analytics	Characterization and Tools	Materials	Processes	Reactor Design	Deployment and Scaling
Hybrid physics/statistics models for capturing non-idealities in dynamic catalyst operation	* (1) Transient modeling tools • Develop the mathematical framework to analyze transient behavior, e.g., resonance	** (2) Smart, switchable materials, e.g., selectivity	“Flexible” processes or forced dynamics		Absolute need for down-scaling, i.e., safety-transport
	Building and operating families of dynamic catalyst HTS screening tools for both discovery and development coupled with data analytics and inferential modeling	* (1) Catalysts for low CO_2 hydrocarbon conversion (low-pressure, low-temperature)	Sensitivity study on quantitative impact of carbon tax on petroleum manufacturing		Availability of renewables (energy, materials) – will spur research on distributed processes that operate near ambient conditions
		Tailored catalysts 100% selective at process temperature			Design catalyst for specific role: distributed, tied to reactive separation
					Retrofit existing units for new catalytic processes

TABLE E-3. ROLES AND COLLABORATION

What are the Roles, and What Collaboration is Needed?			
Follow DOE, EERE, VTO model. Team academia/national labs/catalyst and operating companies	Need collaboration on pre-competitive research	Absorb risk computationally and experimentally at critical decision points through collaboration	Need industry to define toolsets needed, and give frequent feedback (good and bad) on the use of toolsets
Large data synthesis collaboration is needed (industry, academia, government)	Industry performance goal sharing (under NDA?) for directed development projects with sightline to scale up	Standardized data collection and archiving and distribution. Defining “dynamic” test conditions	

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