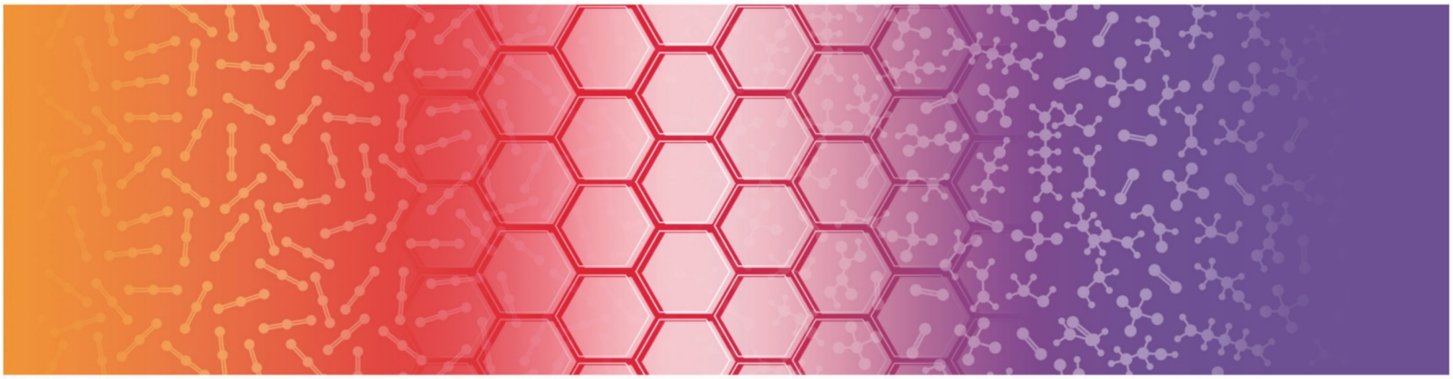

Summary Report of the Reactive CO_2 Capture: Process Integration for the New Carbon Economy Workshop, February 18–19, 2020

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Nomenclature

CAPEX	capital expense
CCS	carbon capture and storage
CCU	carbon capture and utilization
CO_2	carbon dioxide
Gt	gigaton
kg	kilogram
kWh	kilowatt hour
LCA	life cycle analysis
Mt	million tons
OPEX	operating expense
ppm	parts per million
R&D	research and development
RC	reactive capture
TEA	techno-economic analysis
TRL	technology readiness level

Executive Summary

Decarbonization of our global economy is required to limit planetary warming to +1.5ºC above pre-industrial levels, an ambitious goal set into motion by the Paris agreement. Given the scale and urgency, the solution demands international, cross-sector advancements spanning policy, social responsibility, and technology, with emphasis on step changes over incremental changes. To that end, technological revolutions that disrupt the status quo need to be envisioned and enacted.

One potential technological revolution is the production of fuels, chemicals, and materials from carbon dioxide (CO_2) as the starting feedstock, leveraging renewable energy as the driving force. Over the past decades, significant research, development, and deployment has occurred on technologies for capturing CO_2 from point sources or the air and utilizing this CO_2 as a working fluid or as a chemical reactant; however, most of this work has been siloed in these two categories. Recently, an emerging field has started to explore the direct integration of CO_2 capture and conversion technologies as a means to reduce overall energy demand (i.e., avoid energy penalty of CO_2 desorption/regeneration of capture media) and capital expense through process intensification. This strategy represents an opportunity to leapfrog forward this technological revolution. However, the field is in its infancy and the technologies are at an early stage of development, thus it is critically important to define and assess the value proposition of this strategy relative to alternatives (e.g., separated capture and conversion technologies, fuels and chemicals derived from renewable feedstocks like biomass, and industrial electrification) to chart a path forward.

To identify next steps, we organized a workshop titled "Reactive CO_2 Capture: Process Integration for the New Carbon Economy" which was held in Golden, Colorado, February 18−19, 2020. The focus of this workshop was to discuss approaches for merging CO_2 capture and CO_2 conversion/utilization systems into what we denoted as an integrated "reactive capture" strategy. By our definition, reactive capture of CO_2 is the coupled process of capturing CO_2 from a mixed gas stream and converting it into a valuable product without going through a purified CO_2 intermediate (see full definition in the Introduction section).

This report seeks to summarize feedback from the approximately 125 participants and subject matter experts in attendance from academia, industry, U.S. Department of Energy (DOE), and DOE national laboratories. The workshop agenda is included in Appendix A and the full list of attendees can be found in Appendix B. To elucidate a path forward, we first asked the attendees to define what success would look like for reactive capture in the short term (0–5 years), midterm (5–10 years), and long term (10+ years) and then asked them to answer four questions related to how we could achieve that success: (1) What are the key barriers and challenges to success? (2) What are needed activities to overcome barriers and challenges? (3) What opportunities will arise from these activities? (4) What is a target outcome and what metrics need to be met?

By convening these experts at this workshop, we were able to identify four key themes and associated calls to action for the reactive capture community:

- *Essential Role of Partnerships*: While reactive capture is just one technological strategy, we are trying to solve a global, urgent challenge in climate change. Thus, we all need to pull together across academia, government, and industry to accelerate the development of this reactive capture field, first by defining and assessing the value proposition and second by forming teams across the value chain to move from concept to scale-up, with the goal of reaching pilot-scale demonstrations in the next 5–10 years.

- *Critical Challenges*: Key, cross-cutting challenges for reactive capture include: (1) addressing the mismatch in existing rates of CO_2 emission, capture, and conversion processes through process design and scale/rate balancing; (2) developing approaches that are robust under intermittent operation; and (3) identifying locations with availability of CO_2, access to inexpensive, renewable electricity, and proximity to product markets.

- *Defining the Value Proposition:* Existing and emerging experimental datasets on reactive capture technologies need to be integrated with rigorous techno-economic and life cycle analysis and the results need to be assessed in comparison to the status quo as well as alternatives, such as separated capture and conversion. This work needs to be performed early on in the field to identify advantages, limitations, and research and development needs, and experimental, proof-of-concept demonstrations should utilize realistic CO_2 feed streams.

- *Approach to Support Technological Advancement*: The techno-economic and life cycle analysis note above should also help identify promising new routes for reactive capture and define standardized performance metrics for benchmarking and reporting. Guided by this analysis, experimental work should seek to move from a diverse portfolio of emerging reactive capture technologies at technology readiness levels 1–3 to pilot scale (>1 ton per day of CO_2 converted) in the next 5–10 years with a goal of achieving a 30% reduction in cost and 30% improvement in energy efficiency over comparable separated capture and conversion processes.

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1 Introduction

In this century, to avoid the most catastrophic effects of climate change, we must change how we make things, move about, and power the world. Net greenhouse gas—primarily carbon dioxide (CO_2)—emissions from anthropogenic sources must be dramatically reduced by the end of the century to limit planetary warming to +2ºC relative to pre-industrial levels; scenarios limiting warming to +1.5ºC call for zeroing greenhouse gas emissions around mid-century.[1] This requires near-term efforts to reduce the carbon footprint of existing fossil fuel-based processes, and a long-term transition to alternative carbon sources as the primary building block for all other carbon-containing products. It is estimated that a transition from petroleum as a carbon feedstock to CO_2, either as a waste emission or from the air, can eliminate a significant 3.5 gigatons of emissions every year.[2] Establishing a circular carbon economy requires substituting petroleum-based feedstocks with those derived from CO_2, but there are several key challenges:

- There are many sources for CO_2, including exhaust gas from combustion and power generation, CO_2 capture from air, and CO_2 co-produced with biogas, and they vary in scale, concentration, location, and impurity profile. Thus, a singular technology solution may not be possible. Further, the CO_2 capture processes for these streams have high capital and operating expenses (CAPEX and OPEX).

- Converting CO_2 to feedstock molecules or fuels will require large quantities of renewable energy, likely in the form of renewable or carbon-free electricity. It is estimated that if all chemical manufacturing was transitioned to using renewable energy, the majority of the projected buildout of renewable energy in 2030 on the planet would be required.[2]

Ultimately, replacing petroleum-based feedstocks with CO_2-derived feedstocks requires CAPEX and OPEX reductions for both the CO_2 capture and conversion steps as well as a reconsideration of our centralized processing model if this is to be achieved at a meaningful scale. ***This is a massive challenge—process intensification and energy efficiency will be critical drivers to enable a faster transition to the necessary circular carbon economy, where products and fuels are made from waste CO_2 with minimal net emissions.***

1.1 Value Proposition—Reactive Capture

Efforts to establish a circular carbon economy have generally focused on two main research areas: capture of CO_2 from point sources or the air, and separately, CO_2 conversion into fuels and chemicals (see Figure 1). The focus of this report is to identify strategies for merging these CO_2 capture and CO_2 conversion systems into a more integrated "reactive capture (RC)" process. This is a timely effort as a recent National Academies study highlighted reactive separations as a critical research need.[3] Conventional carbon capture and utilization (CCU) approaches assume a sequential path where CO_2 is captured in a carbon capture and storage (CCS) process that produces CO_2 as a high-purity product. CCU processes then react the high-purity CO_2 to make useful products. Reactive capture eliminates the production of high-purity CO_2. The potential benefits of integrated capture and conversion include increased overall energy efficiency and reduced capital expense. In some cases, CO_2 transport costs, and other logistical costs can be eliminated, relative to traditional carbon capture and conversion pathways (see Figure 2). The overall energy efficiency for carbon capture and conversion can be improved because coupling the separation of CO_2 from mixed gas streams directly with a conversion process eliminates the need for capture medium regeneration and CO_2 compression. Regeneration can be accomplished by converting CO_2 into another molecule, and no CO_2 compression is needed. Obviating any need for regeneration and compression steps in carbon capture could potentially eliminate 90% of the power loss (consumption) in a typical amine-based capture process.[4] Additionally, combining unit operations may greatly reduce capital expenditure. An RC process will reduce transportation costs, since the cost of transporting recycled carbon as chemicals will be lower than the cost of transporting CO_2, whether by truck, rail, barge, or pipeline. Of course, the main driver for developing reactive capture technologies is to reduce emissions in a more efficient way, but the development of these new integrated technologies can also provide other environmental co-benefits and geographically distributed economic and employment opportunities.

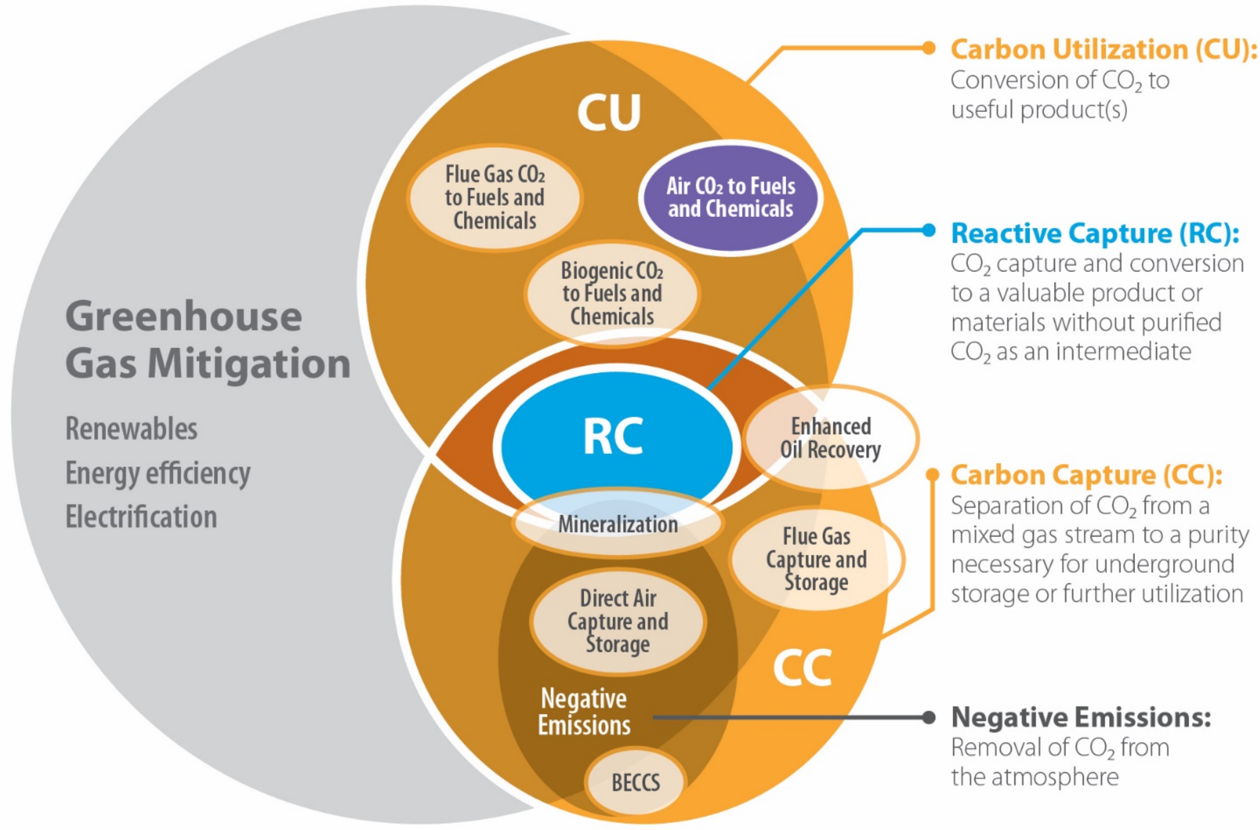

Figure 1. Venn diagram illustrating the relationship of reactive capture strategies (blue) within the broader ecosystem of approaches to capture and utilize CO_2 and mitigate greenhouse gas emissions

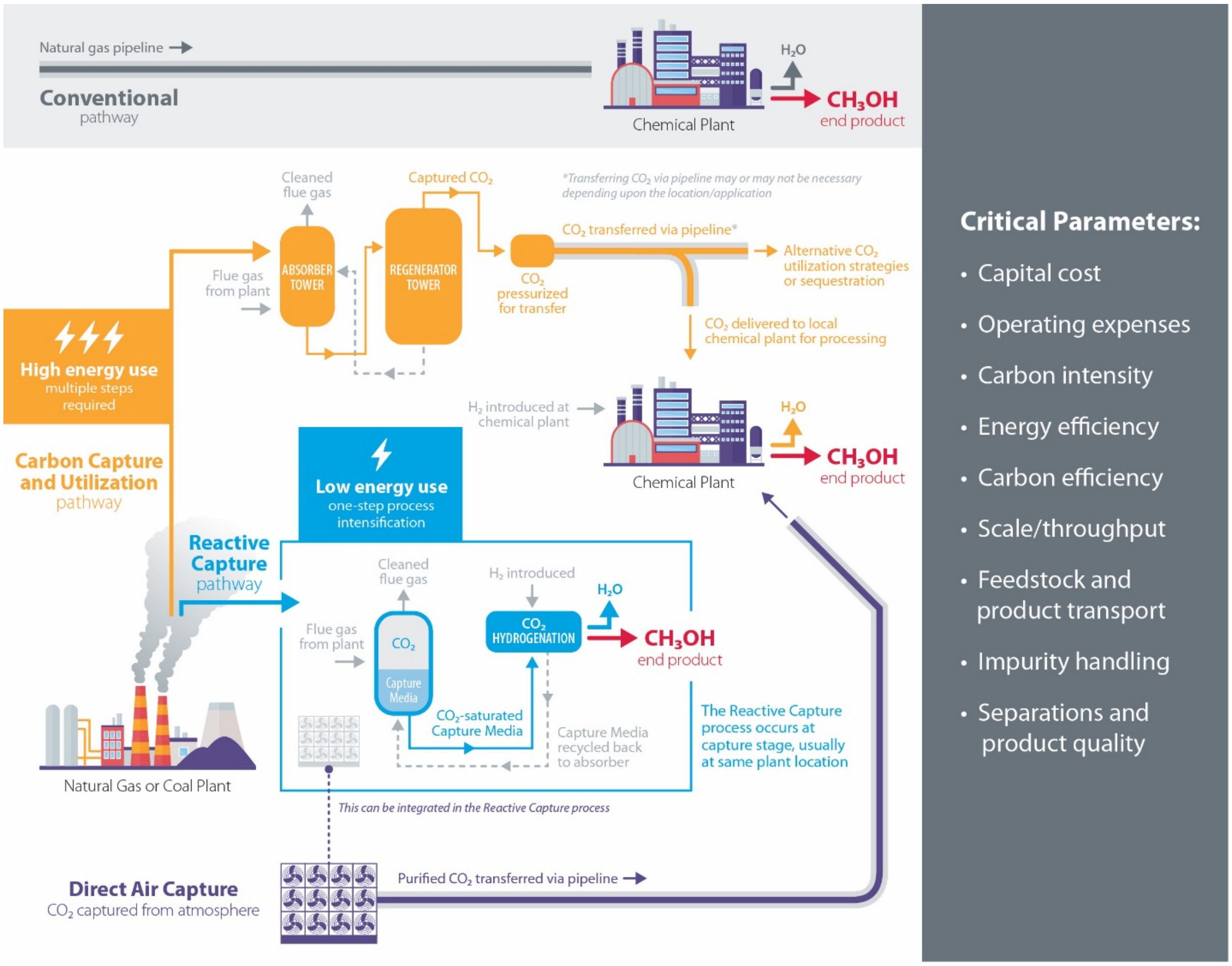

Figure 2. Illustrative example comparing the conventional pathway for methanol production (gray) to RC (blue) and CCU (orange) approaches for transforming CO_2 from a coal-fired or natural gas power plant into methanol. Integration with direct air capture (purple) is also shown.

1.2 Definition of Reactive Capture

For the purposes of the workshop and this report, we defined the term reactive capture as the integration of two processes: the CO_2 separation from dilute gas streams and conversion of CO_2 to valuable product(s) without going through a purified CO_2 intermediate. We defined this "process integration" broadly, as any process that is more integrated than the current state of the two processes, which typically involves a capture unit, an energy-intensive sorbent/solvent regeneration step, and CO_2 compression, followed by feeding pure CO_2 into the conversion unit. For our purposes, reactive capture may comprise the integration of CO_2 separation and conversion in a method using fewer steps, one reactor, or simply process intensification (reduced unit operations) in the pathway from CO_2 in a mixed gas stream to a CO_2-derived product. All levels of process integration would provide potential efficiency and cost benefits relative to the current state of the art. While the coupled/integrated capture and conversion of CO_2 can encompass an expansive set of natural and technological pathways, including production of biomass and a wide range of products, we defined processes that met the reactive capture definition narrowly in this report. Our intent was to focus the discussion on emerging research needs in areas that are not supported by other programs, and on products that have current uses and can potentially provide economic drivers for technology development. We stipulated the process must produce a valuable chemical feedstock/product, or mixture of chemical feedstocks/products, and these products must be in a more reduced state than CO_2 (e.g., we did not consider production of carbonates). Therefore, while mineralization approaches can be considered reactive capture in principle, we did not consider them here. Similarly, we also did not consider processes that rely on photosynthesis for carbon capture and storage. The target CO_2 streams in this report include capture from air (~415 ppm CO_2), exhaust gas from combustion and power generation (4%–14% CO_2), and CO_2 co-produced with biogas (~45% CO_2).

1.3 Need for Workshop and Workshop Goals

In the context of enabling a circular carbon economy by generating fuels and chemicals from waste CO_2 streams, current efforts have generally bifurcated between two camps: CO_2 capture and CO_2 utilization. The distinctions between these two research areas have often resulted in little communication between researchers working on the two fields and with little effort devoted to their co-integration. We had the following goals for this workshop:

- Bring the carbon capture and utilization (conversion) communities together to define and envision the benefits of reactive capture.
- Define success at various time intervals to provide guideposts on the path to full deployment and implementation.
- Identify the technological, as well as logistical, economic, political, and communications barriers that must be overcome to achieve the envisioned successful outcomes.

This report synthesizes the thoughts and discussion from the capture and utilization communities on the needed activities to achieve the targeted outcomes from reactive capture.

2 Workshop Structure and Agenda

This workshop was by invitation only, with the organizers seeking representation from stakeholders in carbon capture and utilization across industry, academia, national laboratories, and several U.S. Department of Energy (DOE) offices. Invitation and registration targeted 30% participation from each of the three sectors with the balance made up of DOE representatives. The goal was to encourage participants to think outside of their sandbox and work across traditional boundaries and participate in constructive dialogue to map a strategy for a hybridized approach of carbon capture and utilization. The agenda (see Appendix A) was structured to define the problem, establish a vision of success, and break out into smaller groups for discussion, consensus, and report-out. The organizers built the workshop around timeframes of short term (0 to 5 years), midterm (5 to 10 years), and long term (10+ years) to bracket the discussions. With the purpose of maintaining balanced representation from the three sectors, the ~125 attendees (see Appendix B for full attendee list) were assigned to one of five breakout groups, and further assigned to one of the three timeframes within that group. All of the five main groups were tasked with answering the same questions.

The first assignment for each group was to further refine and articulate successful outcomes at each of the timeframes. With an eye for achieving those successes, participants were then asked to respond to and discuss specific questions about how such successes could be realized within their assigned timeframes, particularly: (1) What are the key barriers and challenges to success? (2) What are needed activities to overcome barriers and challenges? (3) What opportunities will arise from these activities? (4) What is a target outcome and what metrics need to be met? Additional discussion topics (see Appendix A) were provided to help each group flesh out the responses. Feedback from each breakout room was collected and discussed before all participants regathered for a read-out of the responses to the entire workshop.

2.1 Key Themes

As a result of these exercises, four key overarching themes were identified from this workshop:

Essential Role of Partnerships

Collaboration between partners in academia, government, and industry is critically important, especially in moving from the lab-scale (short-term) to pilot-scale (midterm) phases of technology development. A consortium of various stakeholders should define policy and a diversity of scientific expertise is needed to identify, develop, and implement the technologies. DOE should support preliminary validations of the various components of reactive capture systems and commission technical and economic analyses to identify promising sites for pilot-scale reactive capture demonstrations. DOE should also facilitate partnerships between RC researchers and industries that are producing CO_2.

Critical Challenges

One critical challenge is overcoming the huge mismatch in the existing rates of CO_2 emission, capture, and conversion processes. To effectively couple reactive capture solutions with emissions, the vastly different scale of operations needs to be considered and addressed. There may be a need to build reactive capture systems that are robust under intermittent operation to utilize curtailed or off-peak, renewably generated electrons. The "tri-location" (coined by Opus 12) challenge—the convergence of CO_2 sources, access to (inexpensive/surplus) electricity, and proximity to product markets—can identify the most promising locations for initial implementation. This challenge could also be an opportunity to generate employment opportunities in rural, remote locations.

Setting Relevant Targets and Defining the Value Proposition

There is a need to determine whether the value proposition(s) for reactive capture (relative to sequential capture and conversion) holds; this needs to be done early. The prospects for reactive capture should be evaluated with rigorous techno-economic and life cycle analysis (TEA and LCA) and key figures of merit should be identified. DOE should use these analyses to *target an outcome*, not a process, and be technology agnostic. Pilot-scale testing should be a key milestone in the maturation of reactive capture technologies and used to corroborate TEA/LCA models. TEA/LCA can also be used to identify products with the most economic and/or environmental promise.

Approach to Support Technological Advancement

A significant effort on TEA/LCA is needed to first identify promising new routes and then to validate those routes with data from deployments. Informed policy, combined with technology advancement, will enable rapid advancement in the economic feasibility of reactive capture. We have technologies that work, but at present, these technologies/systems are not economically viable. Funding should target joint projects that include input from national labs, universities, and industrial partners. This will help focus "bench-scale" efforts to meet near- and midterm objectives for deployable technologies. We need to move quickly to identify promising approaches so they can begin to be deployed at the field scale in 5 years.

2.2 Definitions of Success

Attendees at the workshop brainstormed definitions of success at different time horizons, near term (<5 years), midterm (5–10 years), and long term (10+ years). This exercise was intended to help assess the current state of technology, set reasonable, staged goals, and envision the outcomes of those goals.

Near-Term Time Horizon (<5 years)

Existing bench-scale RC technologies have been de-risked with proof-of-concept demonstrations at the kg/h scale. The advantages, limitations, and research and development (R&D) needs for existing RC technologies (in relation to comparable CCU processes) have been identified through comprehensive TEA/LCA. Fundamental RC R&D efforts have resulted in discovery of new approaches, resulting in a diverse portfolio of emerging RC technologies with over 100 peer-reviewed publications. An RC consortium has been established to support the growth of an RC ecosystem.

Midterm Time Horizon (5–10 years)

Technology readiness level (TRL) of RC processes have been advanced to TRL 7 through pilot-scale (i.e., >1 ton per day of CO_2 converted) operations under industrially relevant conditions for at least 5,000 hours of on-stream time, leveraging test bed capabilities established within the RC consortium. RC technologies have achieved a 30% reduction in cost and 30% improvement in energy efficiency relative to comparable CCU processes.

Long-Term Time Horizon (10+ years)

RC is widely accepted as an enabling wedge (potential to achieve 0.5 Gt/year of CO_2 utilization) toward achieving a circular carbon economy. RC technologies are 50% more energy efficient and have 50% lower capital costs than comparable CCU processes. Commercial-scale RC systems are deployed at fossil fuel power plants and have been demonstrated with direct air capture.

3 Challenges, Needs, Critical Activities, Targeted Outcomes, and Recommendations

For each of the time horizons discussed during the workshop, we collected attendee input on four components: (1) key challenges and barriers, (2) needed activities to address barriers, (3) opportunities, and (4) targeted outcomes and key metrics for success. Feedback on these four components for each time horizon is summarized below, concluding with recommended next steps.

3.1 Near-Term Time Horizon (<5 Years)

3.1.1 Key Challenges and Barriers

As described above, we defined near-term success broadly as scaling up and de-risking technologies that are promising today, and creating tools, supporting infrastructure and communication among researchers and stakeholders to pave the way for the next generation of promising technologies. Many technologies are not yet imagined, proven, and de-risked, thus limiting commercial viability. In the next section, we will go over recommendations for overcoming these challenges. The key challenges and barriers to near-term success are not just technological; logistics, communication, and supporting analysis are also lacking.

A major technical concern with demonstrating RC, in relation to the current state of technology for sequential capture and conversion technologies, is an inherent mismatch between scales and rates of capture and conversion. In most cases, carbon capture rates and scales vastly exceed available CO_2 conversion technologies because the former already exist at pilot or pre-commercial scale while most of the latter technologies have only been demonstrated at the lab scale. This mismatch can potentially be addressed by numbering up modular conversion processes. An additional challenge is that sequential capture/conversion process must remove impurities when high-purity CO_2 is produced. Integrated RC systems may need additional steps to address impurities.

Technology demonstrations will require a supportive ecosystem that can help assess the potential benefits of RC, including standardized tools for evaluating economic and environmental impacts. A matured ecosystem for this does not currently exist for RC technologies. However, it is conceivable that many of the broader approaches used in conducting TEA for renewable energy systems and studying the environmental impacts of mitigating CO_2 emissions in general, could be adapted for quantitatively rigorous evaluation of RC systems. For example, aggregating performance metrics such as the volume of CO_2 captured per kWh (or amount of CO_2 converted to product per unit of energy relative to the total amount of CO_2 entering the facility), single-pass CO_2 conversion efficiency, and the ratio of RC process costs to plant revenue/profit, could be envisioned as potential methods for benchmarking RC systems. In the latter case, such a unit measure would be highly dependent on the industrial process being coupled to RC and could, therefore, serve to help target the industries and processes best suited for RC process integration. Similarly, measures commonly used in climatology, including the projected impacts that some system of RC at a particular scale of implementation could have on atmospheric CO_2 concentrations and/or global temperatures within relevant timeframes as set by the

Intergovernmental Panel on Climate Change, could potentially become the standard for evaluating environmental impacts of an RC technology.

The goal of scaling and demonstrating promising RC technologies that exist today brings another major challenge to the fore: the tri-location challenge. The source of dilute CO_2 may be in one location, inexpensive, renewable electricity in another, and optimal product transport or market in yet another location.

3.1.2 Needed Activities to Address Barriers

Near-term success in RC can only be found when the community understands the value proposition, the technical challenges of RC, and how it is distinct from CCS and CCU. This understanding can be gained by facilitating robust cross-disciplinary communication and engagement. Some of the activities to support this communication include creating a consortium of stakeholders to facilitate opportunities, develop policy that is outcome focused, and connect technologists from different backgrounds and sectors. In addition, putting open-access data and resource-mapping in the hands of research and industrial stakeholders will catalyze new projects. These data include CO_2-rich feedstock classification, characterization, and location information. This resource mapping can also be used to identify sites that meet the tri-location challenge, including CO_2 source, energy source and cost, and product distribution modes. Researchers need to know what concentration of CO_2 to target, and what impurities to manage. Additionally, understanding ultimate flow rates and scales will also help direct technology development. Access to systems-level information on current capture and utilization processes may also help spur innovation, giving researchers insights into where the processes might be integrated. Access to baseline TEA/LCA data for potential product streams can help direct research activities. Once the information is gathered, artificial intelligence may provide a route to mine for potential integration opportunities.

Building RC test beds to screen and test technologies in a pre-pilot, simulated industrial environment will help de-risk the technologies, draw industrial engagement, and help researchers find design flaws early when costs are lower. Additional technology development targeted at reducing the cost of CO_2 electrolyzers and increasing systemwide energy efficiency will make the technologies more feasible to pilot. To develop next generation technologies, researchers can pursue an increased understanding of reactivity of CO_2 adducts under catalytic conditions to make favored products, and/or target conversion technologies that occur in CO_2 separation media.

3.1.3 Opportunities

Workshop participants identified new opportunities in the scaling and de-risking activities for existing technologies, as well as opportunities in the development of next generation technologies. For nascent technologies, putting together new, multidisciplinary teams can seed an RC R&D community that can shorten time scale of success. These teams can also work to identify and target high-value products for niche markets to offset risk of early investment, as well as identify new RC chemistries.

De-risking and putting existing RC technologies on path to deployment will generate economic and social benefits. Broadly, the ability to create a revenue stream from capture and conversion of a waste product can change the business case for traditional CCS deployment, especially if the pathway is eligible for government tax incentives such as Section 45Q. From the product perspective, RC provides an opportunity to lower the carbon intensity of existing products by using otherwise emitted CO_2. The product may have additional value for decarbonization if it can be used to store electricity long term. Finally, new RC industries will put carbon back to work in the American economy, creating economic opportunities and jobs in vulnerable areas.

3.1.4 Targeted Outcomes and Key Metrics for Success

Targeted outcomes for the near term can be broadly grouped into four categories: (1) de-risking of technologies, (2) development of a robust research program and portfolio, (3) an improved systems-level understanding of risks and benefits, and (4) demonstrated improvement in information sharing across disciplines.

For de-risking of technologies, a key metric for success is multiple (>10) proof of concept lab-scale demonstrations of RC that can be implemented at pilot scales. We also target a more advanced demonstration within 5 years at kg/day scale that combines processes that are readily integrated chemically and energetically.

A robust research program will have a portfolio of RC technologies that work on laboratory scale, with well-defined R&D benchmarks based on robust systems analysis. A key metric for this research program is 100+ publications on RC in 3 to 5 years.

The improved systems-level understanding will be demonstrated by developing a framework of TEA and LCA that can project economic viability at full scale. These analyses need to be performed not only for RC versus traditional pathways but also for decoupled CC and CU for comparison across all pathways listed in Figure 2.

Demonstrated information sharing will include a multidisciplinary forum/wiki for bringing together issues and solutions in RC.

3.1.5 Near-Term Summary

In the near term, defined as within the next 5 years, the main challenges are around the maturity of the technology and compatibility rates of RC with CO_2 sources, as well as finding suitable locations with intersecting resource availability. Other challenges are differentiating RC from CCS and CCU and a lack of agreed-upon figures of merit as well as standards for technology assessment (TEA/LCA) methods. To address these challenges, RC test beds are needed to screen promising technologies and resource maps should be developed to identify optimal (tri-)locations to facilitate success for the first RC deployments. There is also need for collaboration at many levels; from a consortium of stakeholders to facilitate opportunities and develop policy to connecting technologists from different backgrounds and sectors to solve this multidisciplinary challenge. These collaborative efforts offer the opportunity to seed an RC R&D community to shorten the time scale of success. There are also economic opportunities to turn CO_2 emissions from a liability to an asset while simultaneously creating jobs that could be located in rural areas of the country. A targeted outcome would be to have multiple proof-of-concept lab-scale demonstrations that can be implemented at pilot scales as well as at least one RC technology that has been deployed at the pre-pilot scale. The metrics for success must be defined by developing an agreed-upon framework of TEA/LCA to project economic viability at full scale that also establishes a timeline of what RC R&D technical targets must be met to maintain suitable progress.

Near-Term Recommendations

- Broad support for new, scalable ideas and technologies
- Consensus on figures of merit and appropriate TEA/LCA methodologies to identify sensitivities (research targets) that will yield greatest return on investment
- Identify locations with appropriate resources for first implementations.

3.2 Mid-Term Time Horizon (5–10 Years)

3.2.1 Key Challenges and Barriers

For mid-term success, we target moving promising technologies further toward demonstration and commercialization; these demonstrations must show promising life cycle and economic performance (30% lower emissions and lower costs than the conventional CCU pathway).

The challenges and barriers to achieving this goal include market uncertainties, technical challenges, and supporting policy, partnerships, and infrastructure. Commercial-scale technology deployment requires large capital investment that may take several years to generate a return; investors must have some certainty around the source and consistency of mixed gas feedstock, markets for their products, and government incentives. As it will dictate the economics and overall emissions of the process, the availability of inexpensive renewable energy sources, such as electricity, renewable natural gas, and/or hydrogen, will need to be projected and guaranteed. If the source of energy is intermittent, the capacity factor of the RC process will decrease and thus impact the economics. Determining which specific products to target for the full-scale demonstrations will be critical at the mid-term time horizon. This is challenging with dynamic markets and future uncertainty and may be influenced by public perception of product from waste CO_2. On the technical side, similar to the near-term challenges, matching rates of capture with rates of conversion in a continuous process will be challenging, particularly at increasing scales and economic requirements for both processes.

Appropriate risk assessment and management will require long-term operational data and durability testing protocols, as well as testing on real gas streams, to inform further piloting and permitting processes.

3.2.2 Needed Activities to Address Barriers

The RC processes must be rigorously tested to understand and manage risk; these activities include operating RC pilot tests for long durations with industrially relevant inputs to validate CAPEX and OPEX assumptions. Additionally, the pilot tests are needed for the development of TEA/LCA models. These TEA/LCA models must be developed with vetted standards to support and attract industrial confidence and investment. Beyond economic and emission assessments, early adopters should be encouraged with incentives and a support system. These activities may include process demonstration laboratories with engineering support for validation. Validation activities can include research on integration across length, time, and flow scales, as well as evaluating and, if necessary, overcoming the effects of intermittency with a "warm standby" mode. Early adopters need to be supported with start-up incubators (e.g., Greentown Labs and Cyclotron Road-type efforts), as well as education of the public and policymakers on the challenges and societal benefits of the technologies.

3.2.3 Opportunities

The research and development activities outlined above will provide an opportunity for new understanding and, potentially, the discovery of new breakthrough chemistries and technologies. For example, R&D activities will lead to new chemistries for monomers and chemicals that build on bound CO_2 that may have novel, improved functionality. These activities will also shed light on process flexibility to take new waste gas streams or produce a different product, which may be necessary as markets change. The research activities will provide new routes of capturing and activating CO_2; these may allow electrification of parts or the entire process. Scientific understanding of degradation and durability including learning what we do not know, can potentially be applied more broadly. Lessons learned from scale-up and integration will provide information to build full-scale plants, which will increase investment consideration. There could be new avenues and opportunities for collaboration such as targeted collaboration between academia, national labs, and industry to accelerate technology development, scaling, and commercialization efforts. Successfully reducing the time to market will be crucial for establishing stakeholder/public support and wider industrial interest. Enhanced visibility, improved public perception, market tests, and job creation are additional opportunities.

3.2.4 Targeted Outcomes and Key Metrics for Success

Demonstration of one or two RC processes at pilot scale that have performance enhancement over conventional CCU processes will confirm success. These pilot RC processes must operate at reasonable scale (e.g., a suggested scale is 1 ton per day of CO_2 converted) with realistic inputs. This process must have demonstrated durability on the order of 5,000 hours. The results of the demonstrations show a path to economic viability in a vetted TEA. In conjunction, the innovation ecosystem provides stable policy to allow for mid-term investment.

3.2.5 Mid-Term Summary

In the mid-term time horizon, defined as 5–10 years from now, the key challenges are related to risk assessment and management. The uncertainty in markets and incentives for CO_2 use makes the choice of an optimal product to target unclear. The main technological hurdle is matching the RC rates with CO_2 sources to make RC a continuous, rather than batch, process. Running RC pilot tests for long durations should validate assumptions and increase confidence in TEA/LCA models to encourage and support industrial investment. In addition to supporting research on integration across length, time, and flow scales, there should also be policy developed to incentivize early adopters of RC technologies. The new approaches available in RC are an opportunity to choose new chemistries and products that may have novel functionality and flexibility compared with traditional chemicals from established, inflexible processes. The investment in RC technologies also offers opportunities for new collaborations, enhanced visibility, improved public perception, market tests, and jobs. To be considered a success, there should be an RC demonstration of an integrated process that has improved performance over the conventional CCU process and works at scale with realistic inputs. Having one or two pilot-scale RC plants that demonstrate a process is durable in a real system should validate the TEA/LCA and show a path to economic viability.

Mid-Term Recommendations

- Use more advanced and vetted TEA and LCA, informed by pilot-scale experience, to de-risk RC technology approaches
- Support research that seeks to match the rates of RC with emissions
- Implement policy and incentives that encourage early adopters.

3.3 Long-Term Time Horizon (10+ Years)

3.3.1 Key Challenges and Barriers

The long-term vision is that RC has a meaningful impact on enabling a circular carbon economy (0.5 Gt/year wedge) and is economically viable. This means that the fundamental research discoveries made today in this nascent field are carried all the way to large-scale application. The barriers include those identified for near- and mid-term time horizons. Barriers to the scale of operation necessary to enable a circular carbon economy are many, and include *lack of existing supply chains* (e.g., carbon capture media, specialized solvents, membranes, and catalysts) and logistics that will be required to support deployed technologies, such as streamlined permitting, guaranteed waste gas reactant streams, and economical product transport and distribution. At millions of tons of CO_2, or greater, deployment, public perception, market uncertainty, and policy uncertainty could prevent investment.

3.3.2 Needed Activities to Address Barriers

For large-scale deployment, new, distinct activities are needed. A workforce with sufficient training to install and operate the plant must be available in the (potentially more remote) location. Some degree of automation will be necessary at this scale, and automation of new processes must be developed, especially regarding energy intermittency, temporal changes in impurity profiles, and matching capture and conversion rates. Startup companies may serve to fill supply chain needs to facilitate large-scale implementation of the technology.

RC plants or additions to existing plants will likely require tens of millions of dollars of investment, and likely much more, depending on the scale. Therefore, reliable TEA, market research, and long-term financing models and incentives must be available. Geospatial models will be required to identify viable sites for the RC plant, and if the RC process is sited far from the waste gas source, the RC technologies will need to be able to adapt to changing point sources.

Attendees emphasized that long-term policies that encourage RC should be focused only on a carbon utilization and economic outcome instead of specifying the RC pathway.

The need for market pull (at a very large scale) requires that the public has awareness and a favorable view of products made from waste CO_2. This could be accomplished through some certification/validation process (e.g., certified organic and energy star).

3.3.3 Opportunities

The opportunities in RC center around the promise of the new carbon economy: RC may generate new industries, business opportunities, and jobs in vulnerable communities. If RC does in fact reduce carbon capture and conversion costs due to process intensification and integration, more tons of carbon will be utilized per dollar, and RC will have a greater environmental impact than if the processes were not integrated. Since RC stores energy via CO_2, increased energy storage will reduce curtailment, increase deployment of new renewable energy generation capacity, and decarbonize sectors that are difficult to electrify. The use of CO_2 as a carbon feedstock will reduce the need to extract fossil fuels and could have myriad air quality and other human health benefits from their reduced extraction and combustion.

Innovation hubs developed with multidisciplinary teams across different sectors and industries can be a model for solving other emerging, global-scale problems. In particular, RC provides a unique opportunity for cross-disciplinary collaboration between industries, including the chemical and energy industries.

3.3.4 Targeted Outcomes and Key Metrics for Success

The broad targeted outcome of an RC industry is the major reduction in carbon intensity of products, including the replacement of the highest carbon intensity fossil fuel derived products, to increase the rate of decarbonization in the United States and around the globe. To achieve this outcome, RC must be deployed at scale (150 Mt–0.5 Gt)/year and become a core a technology platform for the circular carbon economy. This can be possible if RC can be developed to be more energy efficient, cheaper, and faster to market than traditional carbon capture and utilization processes. The United States has an opportunity to lead this industry, and impact global emissions by serving as a proving ground for the international community.

3.3.5 Long-Term Summary

In the long term, or beyond 10 years from now, the key challenges are de-risking RC technologies at commercial scale and developing the supply chains to support a robust RC industry. The other challenges are accelerating the incorporation of fundamental research discoveries into applications at scale, ensuring that RC technologies are versatile enough to accommodate changes in future point source rates and compositions, and maintaining public awareness of the value of RC. To address these challenges, we need companies to identify and fill these new supply chain demands to facilitate large-scale RC implementation. Continued de-risking through TEA, market research, and financing models should keep investment in RC flowing. Other barriers can be addressed through long-term policy supporting RC that is outcome-, instead of pathway-, oriented, as well as a certification process to maintain public confidence in, and awareness of, RC. Several economic opportunities can be realized through the adoption of RC at scale with new industries, enterprises, and jobs being created, especially in rural communities that can support remote deployment. The energy storage in chemical bonds can enable increased deployment of renewable energy generation by reduced curtailment and help decarbonize sectors that are difficult to electrify. The innovation hubs developed to address RC can be a model for bringing diverse scientific backgrounds and sectors together to solve global-scale challenges facing society that have yet to be identified. To be considered a success, in 10 years RC needs to be deployed at scale and be considered a platform for enabling a circular carbon economy. RC should also yield profitable business ventures that significantly reduce the carbon intensity of at least one fossil-derived product. These outcomes should establish the United States as a leader in RC and provide opportunities for developing countries to implement RC technologies.

Long-Term Recommendations

- Incentivize and support development of supply chain to enable at-scale RC
- Continued de-risking of RC economics through advanced TEA and mature RC facilities
- Establish long-term policy that is outcome-based and implement certification processes to encourage public participation and acceptance.

4 Conclusions

Reactive CO_2 capture—the integration of CO_2 capture and CO_2 conversion systems into a single process without going through a purified CO_2 intermediate—has the potential to serve as an enabling technology wedge toward decarbonizing our economy. However, the reactive capture field is in its infancy and the technologies are only at the proof-of-concept stage, often being demonstrated only at the lab scale with pure CO_2 or simulated CO_2 feed streams. By convening over 100 subject matter experts across academia, industry, and government, our "Reactive CO_2 Capture: Process Integration for the New Carbon Economy" workshop resulted in key calls to action for this community and identified a path to deployment over the next 15 years. Owing to the emerging nature of this field, the critical first steps are to (1) define and assess the value proposition of reactive capture relative to alternatives with the support of TEA and LCA, (2) identify key performance metrics to enable benchmarking, and (3) build a portfolio of technologies, guided by TEA and LCA, through academic, industry, and government partnerships.

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Appendix A: Workshop Agenda and Discussion Topics

February 18, 2020

9–11 a.m.	Optional Tour of NREL Campus

Afternoon Session: Framing the State of the Energy Landscape and Opportunities for Reactive Capture

12:30 p.m.	Check-In and Networking
1 p.m.	Meeting Kickoff Presentation: Peter Agbo (LBNL), Sarah Baker (LLNL), Todd Deutsch (NREL), Doug Kauffman (NETL), and Josh Schaidle (NREL) “Reactive CO2 Capture: Process Integration for a New Carbon Economy”
1:15 p.m.	Presentation: Bill Tumas (NREL) and Roger Aines (LLNL) “Benefits and Challenges for CO_2 Capture and Utilization: The Need for Integration”
2:05 p.m.	Presentation: Sean Simpson (LanzaTech) “Carbon Recycling: Delivering Fuels and Chemicals Using Above Ground Carbon Sources”
3:20 p.m.	Panel Discussion: What Does Success Look Like? What Knowledge Gaps Exist?
5 p.m.	Break/Poster Session Set-Up
5:30–8 p.m.	Reception and Poster Session

February 19, 2020

Morning Session: Technical Presentations on Carbon Capture and Carbon Utilization (with a focus on challenges and opportunities in moving toward integration)

7 a.m.	Breakfast
8 a.m.	Carbon Capture Presentation: David Miller (NETL) “CO_2 Capture Systems and Opportunities for Process Intensification”
8:35 a.m.	Carbon Capture Presentation: David Heldebrant (PNNL) “Exploring the Chemical Synergies Between Capture and Conversion of CO_2”
9:20 a.m.	Carbon Utilization Presentation: Etosha Cave (Opus 12) “Integrating CO_2 Utilization into a Full System: Exciting Opportunities for New Innovation”
9:55 a.m.	Carbon Utilization Presentation: Matt Kanan (Stanford) “Acid-Based Chemistry for Integrated CO_2 Capture and Conversion”
10:25 a.m.	Break and Organize into Breakout Sessions
11 a.m.	Breakout Sessions
12 p.m.	Lunch

Afternoon Session: Moderated Breakout Session Discussions

1 p.m.	Breakout Sessions
3:15 p.m.	Breakout Session Read-Outs
4 p.m.	Closing Remarks
4:15 p.m.	Meeting Adjournment

Additional Discussion Topics

1. What are the challenges of integration when starting with atmospheric versus point sources?
2. For a given mode of capture (e.g., physical sorbent, aqueous, and biological), what specific challenges exist for downstream integration with utilization?
3. For a given mode of conversion (e.g., biological, thermochemical, electrochemical, and hybrid), what specific challenges exist for upstream integration with capture and downstream integration with existing infrastructure?
4. What are the major knowledge gaps and barriers to progress in either capture, conversion, or combined reactive capture?
5. What are current barriers to progress in reactive capture and what research needs to be conducted to address them?
6. Are there any promising bench-scale examples of integrating capture and utilization? How practical and scalable is the technology?
7. Are there products we should target? If so, which ones and why? Products could be fuels, chemicals, or materials.
8. What can we and should we start doing right now to accelerate technological advancement and implementation of reactive capture solutions in the market?
9. Ten years into the future, reactive capture has failed to be implemented at any meaningful scale. What do you believe to be the main technical causes for that failure?

Appendix B: Registered Attendee List

Last Name	First Name	Title	Organization
Ackiewicz	Mark	Director	Division of CCUS R&D
Agbo	Peter	Staff Scientist	Lawrence Berkeley National Laboratory
Aines	Roger	Energy Program Chief Scientist	Lawrence Livermore National Laboratory
Alba-Rubio	Ana	Assistant Professor	University of Toledo
Baker	Sarah	Staff Scientist	Lawrence Livermore National Laboratory
Berben	Louise	Professor	University of California Davis
Bielenber	Jim	Senior Research Associate	ExxonMobil
Billimoria	Rustom	Technical Advisor	ExxonMobil
Braun	Robert	Associate Professor	Colorado School of Mines
Brennecke	Joan	Professor	University of Texas at Austin
Brickett	Lynn	Carbon Capture Program Manager	DOE – Fossil Energy
Brix	Todd	CEO	OCO
Burdyny	Thomas	Assistant Professor	Delft University of Technology
Carpenter	Alberta	Senior Researcher	National Renewable Energy Laboratory
Cave	Etosha	Co-Founder	Opus 12
Chou	Katherine	Staff Scientist	NREL
Circucci	John	Adjunct Research Professor	ASU
Claure	Micaela Taborga	Researcher	ExxonMobil Research & Engineering
Cooper	Jason	Research Scientist	Lawrence Berkeley National Laboratory
Cortright	Randy	Senior Research Associate	NREL
Cresko	Joe	Chief Engineer	DOE EERE
Custelcean	Radu	R&D Staff	Oak Ridge National Laboratory
Dam	Bernard	Dept. Head	TU Delft

De Luna	Phil	Program Director	National Research Council Canada
Deutsch	Todd	Senior Scientist	NREL
Digdaya	Ibadillah	Research Scientist	Caltech
Dowe	Nancy	Senior Scientist - Bioprocess Development	NREL
Duoss	Eric	Group Leader	Lawrence Livermore National Laboratory
Feaster	Jeremy	Postdoctoral Researcher	Lawrence Livermore National Laboratory
Ferrell	Jack	Research Engineer	NREL
Fout	Timothy	Carbon Capture Technology Manager	DOE/NETL
Freeman	Charles	Group Leader – Advanced Energy Systems	Pacific Northwest National Laboratory
Gaffney	Anne	Chief Science Officer	INL
Geerlings	Hans	Principal Research Scientist	TU Delft/Shell
Goeppert	Alain	Research Scientist	Loker Hydrocarbon Institute, USC
Gorski	Christopher	Associate Professor	Penn State University
Gupta	Aalo	Director, Future & Renewable Fuels	Phillips 66
Gupta	Raghubir	President	Susteon Inc.
Hahn	Christopher	Associate Staff Scientist	SLAC National Accelerator Laboratory
Harrison	Keven	Program Manager	NREL
Harvey	Albert	Program Manager Dense Energy Carriers	Shell International
Hatton	T Alan	Professor	MIT
Haynes	Chad	Dir. of Government Strategy	LanzaTech
Heldebrant	David	Chief Scientist	Pacific Northwest National Laboratory
Herder	Paulien	Professor	Delft University of Technology, NL
Hopkinson	David	Technical Portfolio Lead for Carbon Capture	NETL
Jack	Joshua	Research Associate (Postdoctoral)	Princeton University
Jackson	Greg	Professor	Colorado School of Mines
Jiao	Feng	Associate Professor	University of Delaware

Jones	Andrew	Project Manager	DOE
Kanan	Matthew	Associate Professor	Stanford
Kauffman	Douglas	Research Chemist	National Energy Technology Laboratory
Kee	Robert	Professor	Colorado School of Mines
Kenis	Paul	Professor	University of Illinois
Kent	Ronald	Manager, Advanced Technologies	Southern California Gas Company (SoCalGas)
Kidder	Michelle	R&D Scientist	Oak Ridge National Laboratory
Klembara	Melissa	Technology Manager	DOE
Kortlever	Ruud	Assistant Professor	Delft University of Technology
Krause	Ted	Chemical Engineer/Theme Leader	Argonne National Lab
Kumar	AMishi	Program Manager	DOE
Kusuma	Victor	Sr. Research Engineer	LRST/NETL
Lee	Geonhui		University of Toronto
Lee	Uisung	Energy Systems Analyst	Argonne National Lab
Lewnard	Jack	Program Director	DOE – ARPA-E
Lin	Haiqing	Associate Professor	University at Buffalo
Lin	Jerry	Regents Professor	Arizona State University
Lin	Yupo	Technical Group Lead	Argonne National Lab
Liu	Cong	Assistant Chemist	Argonne National Lab
Liu	Di-Jia	Senior Chemist	Argonne National Lab
Long	Jeffrey	Professor	University of California, Berkeley
Marin	Christopher	Research Scientist	NETL/Battelle
Masel	Rich	CEO & Founder	Dioxide Materials
Matuszak	Daniel	Program Manager	DOE Office of Science
Matuszewski	Michael	President	AristoSys LLC
Mihalcea	Christopher	Director New Applications	LanzaTech
Miller	David	Senior Fellow	National Energy Technology Laboratory

Miranda	Raul	Program Manager	DOE
Neale	Nathan	Senior Scientist – Group Manager	NREL
Neyerlin	KC	Senior Scientist	NREL
Nguyen Phan	Thuy Duong	Principal Research Scientist	NETL/Leidos Research Support Team
Nikolic	Heather	Research Program Manager	University of Kentucky Center for Applied Energy Research
Noble	Richard	Research Professor	University of Colorado
Palou-Rivera	Ignasi	Technology Platform Director	RAPID Manufacturing Institute
Pang	Simon	Materials Scientist	Lawrence Livermore National Laboratory
Peretti	Kathryn	AAAS S&T Policy Fellow	Department of Energy
Ping	Eric	Director of Technology	Global Thermostat
Powell	Joe	Chief Scientist – Chemical Engineering	Shell
Ramirez	Andrea	Professor	Delft University of Technology
Rau	Greg	Co-Founder	Planetary Hydrogen
Ren	Jason	Professor	Princeton University
Resch	Michael	Research Scientist	National Renewable Energy Laboratory
Rodrigo Quejigo	Jose	Scientist Biotechnology	Electrochaea
Rowe	Ian	Technology Manager	DOE
Ruth	Mark	IS&F Analysis Group Manager	NREL
Sant	Gaurav	Professor/Director	UCLA
Sarkar	Amitava	Corporate Research Scientist for North America	Total SA
Schaidle	Josh	Research Engineer	NREL
Selman	Nancy	VP Business Development	Skyre, Inc.
Senanayake	Sanjaya	Staff Scientist: Chemist	Brookhaven National Lab
Shin	Youngho	Principal Process Development Engineer	Argonne National Lab
Sick	Volker	Professor	University of Michigan
Simmons	Blake	Division Director	Lawrence Berkeley National Laboratory

Simpson	Sean	CSO, Founder	LanzaTech
Singer	Steven	Senior Scientist	Lawrence Berkeley National Laboratory
Skone	Tim	Sr. Environmental Engineer	U.S. DOE, NETL
Smith	Wilson	Senior Scientist	NREL
Springs	Jerry	R&D Director	Johnson Matthey
Stechel	Ellen	Co-Director and Professor of Practice	ASU LightWorks
Stolaroff	Joshuah	Carbon Capture Technology Manager	Lawrence Livermore National Laboratory
Sun	Xin	Division Director	Oak Ridge National Laboratory
Tao	Ling	Sr. Engineer	National Renewable Energy Laboratory
Trevino	Martha Arellano	Postdoctoral Researcher	NREL
Tsotsis	Theo	Professor	University of Southern California
Tumas	Bill	Associate Lab Director	National Renewable Energy Laboratory
Urgun-Demirtas	Meltem	Group Leader/Lab Relationship Manager	Argonne National Lab
van de Lagemaat	Jao	Center Director	NREL
Verma	Sumit	Researcher-Dense Energy Carriers	Shell
Vickers	James		DOE
Wang	Haotian	Assistant Professor	Rice University
Weber	Adam	Scientist	Lawrence Berkeley National Laboratory
Wilke	Todd	Director Advanced Development	Carbon Engineering
Winkel	John		AMO
Wong	Andrew	Postdoctoral Fellow	Lawrence Livermore National Laboratory
Xiang	CX	Staff Scientist	Caltech
Zelikova	Jane	Chief Scientist	Carbon180
Zhou	James	Senior Director	Susteon

For more information, visit: nrel.gov//bioenergy/workshop-reactive-co2-capture-2020-proceedings.html