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Kolmetz Handbook of Process Equipment Design

CARBON CAPTURE AND STORAGE

(ENGINEERING DESIGN GUIDELINES)

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INTRODUCTION

Scope

Carbon capture and storage (CCS) refers to a collection of technologies that can combat climate change by reducing carbon dioxide (CO_2) emissions. CCS technology is a form of carbon sequestration that's set to play a central role in helping us reach net zero by 2050. Existing strategies to tackle climate change focus mainly on eliminating the carbon emissions from processes such as power generation or transport; but CCS looks at how carbon dioxide (CO_2) can be captured directly from the atmosphere, or at point of emission, and stored safely within the natural environment.

The idea behind CCS is to capture the CO_2 generated by burning fossil fuels before it is released to the atmosphere. Most current CCS strategies call for the injection of CO_2 deep underground. This forms a "closed loop", where the carbon is extracted from the Earth as fossil fuels and then is returned to the Earth as CO_2.

CCS is sometimes referred to as CCUS, where the "U" stands for utilization. Enhanced oil recovery (EOR) is the major use of CO_2 today. EOR is where CO_2 is injected into active oil reservoirs in order to recover more oil. Other possible uses of CO_2 include making chemicals or fuels, but they require large amounts of carbon-free energy, making the costs too high to be competitive today. For large-scale implementation of CCS, utilization is projected to use less than 10% of the captured CO_2.

Carbon capture, utilization, and storage (CCUS) is a promising pathway to decarbonize fossil-based power and industrial sectors and is a bridging technology for a sustainable transition to a net-zero emission energy future. CO_2 storage is a proven and effective way to permanently isolate captured CO_2 from atmosphere. The technical risks associated with CO_2 storage can be managed effectively. Regulatory, oversight, robust site assessment and component site operations support risk management and contribute to CO_2 security.

This guideline provides an overview of process systems engineering (PSE) research challenges, advances, and opportunities for CCUS applications. We review PSE methods, tools, and techniques in process modeling, simulation, optimization, control, material screening, strategic planning, and supply chain network design for CO_2 management. We also attempt to give a PSE perspective on emerging CCUS research interests in molecular and materials systems engineering, multiscale modeling and optimization, systems design and integration under uncertainty, and the application of intelligent systems. The purpose is not to cover all aspects of PSE research for CCUS but rather to foster discussion by presenting some plausible future directions and ideas.

General Design Consideration

Carbon capture, use, and storage (CCUS) is the process of capturing carbon dioxide (CO_2) emissions from fossil power generation and industrial processes for storage deep underground or re-use. CCUS refers to a suite of technologies that can play a critical role in meeting global energy and climate needs. CCUS involves the capture of CO_2 from large point sources and transportation by pipeline, ship, rail or truck to be used in a range of applications, such as enhanced gas recovery (EGR), which traps CO_2 for permanent storage. CCUS technologies will play an important role in meeting net zero targets, including being one of few solutions to tackle emissions from heavy industry.

Capture generally takes place at large stationary sources of CO_2, like power plants or industrial plants that make cement, steel, and chemicals. Most current carbon capture projects use a liquid to chemically remove the CO2 before it goes out the smokestack, but several new types of capture processes are under development.

The captured CO_2 gas is then compressed so it becomes liquid-like and transported to a storage site, generally through a pipeline. Ship transport is more expensive than using pipelines, but it is being considered in both Europe and Japan. Once at the storage site, the CO_2 is pumped more than 2,500 feet down wells into geological formations like used-up oil and gas reservoirs, as well as formations that contain unusable, salty water.

The main use for CO2 today is enhanced oil recovery: pumping CO_2 into oil wells to help flush out hard-to-extract oil. Pure CO2 is also used in greenhouses to grow plants. Most CO2 used for these purposes today is extracted from the earth, but captured CO_2 works just as well.

CO_2 could also be made into useful products. Companies and labs are working on turning CO_2 into plastics, building materials like cement and concrete, fuels, futuristic materials like carbon fibers and graphene, and even household products like baking soda, bleach, antifreeze, inks and paints. Some of these products are already being sold, but none in very large amounts.

Or we could use the CO_2 to grow algae or bacteria. This can then be the basis for making biofuels, fertilizers, or animal feed.

Capturing CO_2 from the air

There has also been considerable interest recently in using CCS technologies to remove CO_2 from the atmosphere. One option is bioenergy with CCS (BECCS), where biomass (like wood or grasses) removes CO_2 from the air through photosynthesis. The biomass is then harvested and burned in a power plant to produce energy, with the CO_2 being captured and stored. This creates what is called "negative emissions" because it takes CO_2 from the atmosphere and stores it.

Another negative emission option is called direct air capture (DAC), where CO_2 is removed from the air using a chemical process. However, the concentration of CO2 in the air is about 300 times less than in the smokestacks of power plants or industrial plants, making it much less efficient to capture. Because of this, DAC is quite expensive today.

CCS takes two basic forms:

- Biological carbon capture and storage: when the natural environment – such as forests and oceans – sequesters CO_2 from the atmosphere.
- Artificial / Geological carbon capture and storage: when CO_2 as an emission is extracted from human-made processes and is stored in vast underground facilities.

Biological CCS happens on a much larger scale than geological CCS, but the technology to stimulate both has traditionally been viewed as expensive and unpractical at scale. This is changing, however, as investment and research into carbon capturing technologies takes off.

Types of carbon capture technology

1. Carbon sinks

   Natural forms of CCS are called ‘carbon sinks’ and they are vast spaces where the natural habitats capture CO_2 from the atmosphere – these include forests, oceans, grasslands and wetlands.

   Scientists, as well as environmental and conservation experts, recognise that the preservation and cultivation of carbon sinks could increase the amount of carbon taken from our atmosphere in the shortest space of time.

   Grasslands and wetlands in particular have a much quicker turnaround for carbon storage, with coastal wetlands storing more carbon per hectare than other habitats like forests.

   Where woodland is used, experts believe certain types of tree - such as birch or willow – are optimal for land-based carbon capture as they absorb more CO_2 comparatively than other tree species.

2. Saline aquifers

   Deep saline aquifers are underground geological formations; vast expanses of porous, sedimentary rock, which are filled with salt water. CO_2 can be injected into these and stored permanently – in fact, saline aquifers have the largest identified storage potential among all other forms of engineered CCS.

   The ‘Endurance’ aquifer, located in the North Sea off the coast of the UK, is one such formation, which sits approximately 1 mile (1.6km) below the sea bed. Roughly the size of Manhattan Island and the height of The Shard or the Empire State Building, its porous composition allows for carbon dioxide to be injected into it and stored safely for potentially thousands of years.

   In the US, multiple large-scale saline aquifers are now being used for CCS purposes, such as the Citronelle Project in Alabama. During its three-year trial period, it was successful in storing more than 150,000 tonnes of CO_2 per year, which was captured from a nearby pilot facility.

3. Giant air filters

   Carbon capture technologies are still being developed globally, with individual countries creating strategies that respond to their own net zero goals. For example, in China companies have developed experimental commercial air filters – huge towers that clean air of pollutants on a huge scale. These giant air towers purify air by drawing it into glass rooms, which are heated using solar power creating a greenhouse effect. This hot air up is pushed up the tower through a series of filters, before being released back into the atmosphere as clean air.

   One such giant air-purifier tower in Xian has reportedly been cleaning more than 353 million cubic feet of air each day, dramatically improving local air quality. Manufacturers believe they are close to developing even larger towers, where just one could clean enough air on a daily basis for a small city.

4. Ionic liquids: a capturing carbon technology of the future?

   The most recent advancements in CCS technology includes new types of liquids, which are highly effective at absorbing CO_2. Two dimensional ‘ionic’ liquids have a molecular structure that allow for higher rates of CO_2 to be absorbed. Scientists believe ‘editing’ liquids can offer more precise control in the chemical engineering process and are considered environmentally friendly.

Planting trees or developing wetland areas are two of the simplest ways of stimulating CCS on huge scales, but there are often issues around land ownership and space. Governments, landowners and local communities all have a role to play in identifying opportunities for projects and collaboration.

Considered the main cause of global warming, carbon dioxide is a topic of great academic and industrial interest. The number of activities emitting this gas tends to grow in the future and they emphasize that not only countries with large economies should adopt reduction measures, but every country should employ environmental policies aimed at mitigating them.

To address the control of carbon dioxide emissions, several R&D&I efforts are conducted in order to mitigate this gas emission. Point out that its use can be divided into four categories:

1. Chemical production (e.g., raw material for polymers and carbonates).
2. Fuel production (e.g., raw material for gasoline and diesel).
3. Biological exploitation (e.g., source of C for microalgae growth).
4. Conventional use (e.g., solvent).

Cites as carbon dioxide mitigation processes: more efficient use of energy, replacement of fossil fuels with others with less carbon content, use of energy solutions that use renewable energy sources and storage of carbon dioxide in geological formations.

Among the alternatives for mitigating carbon dioxide, its use as a raw material represents an option of great economic and environmental appeal, as it allows its use as an input in industrial processes and can collaborate in the formation of innovative products and materials. Characteristics such as abundance, low toxicity and low cost, make carbon dioxide an excellent raw material . Aiming its capture for industrial usages, the technologies are directed to capture this gas in the purest, economical and environmentally viable way. The carbon dioxide capture can be carried out during three stages (Intergovernmental Panel On Climate Change, 2005):

- Pre-Combustion
- Combustion
- Post-Combustion

Pre-combustion is based on a gasification process through which the fuel passes and is intended to produce a synthesis gas, mainly composed of hydrogen and carbon monoxide.

Subsequently, hydrogen and carbon monoxide are converted into carbon dioxide and then this goes through the gas separation process.

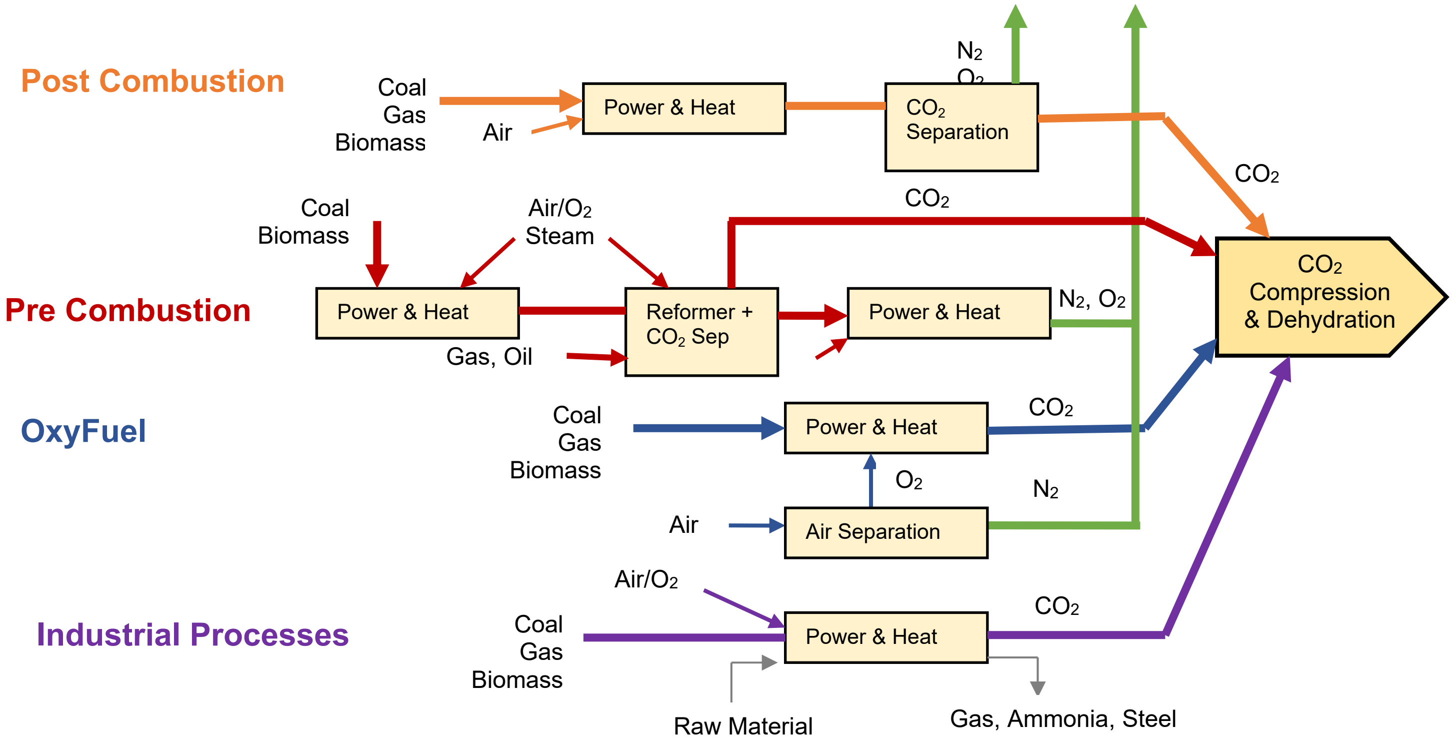

Figure 1. Overview of CO_2 Capture Process and System

The capture of gases that occurs during combustion is called oxy-combustion or oxyfuel and its principle is the burning of fuel in an oxygen-enriched environment.

Post-combustion is the capture in the final phase of release of the combustion gases. It is ideal for capturing CO2 from energy generation sources, such as thermoelectric plants and other plants that use waste to generate energy. After the combustion gases exit, they go through the process of separating CO2 from the other gases using the appropriate technology.

Defining the stage at which gas capture will occur is essential for defining separation technologies. Since these two factors are directly related, it is possible to provide the best technology that meets the criteria of cost, deployment, time, purity and abundance of CO_2. In the next session we will discuss the main categories of carbon dioxide separation technology.

PROCESS DESIGN, SYNTHESIS AND OPTIMIZATION

Many researchers investigated several CCUS process designs and syntheses based on different capture technologies (liquid chemisorption, solid adsorption, calcium looping), capture from different source streams (e.g., electric power generation, post-combustion, oxy-fuel combustion, pre-combustion), capture from industrial plants (e.g., iron and steel plant, cement production, petroleum refineries, hydrogen production, ethanol plants), capture from air (using liquid solvent, solid sorbent), several sequestrations (e.g., deep geological formation, carbon mineralization), potential CO_2 utilization (e.g., chemical production, fuels, concrete and building materials, EOR, bioenergy, geothermal energy) and possible transport and compression options. Some key works that employed the PSE technique for the design and synthesis of various CCUS supply chain components.

MATERIAL SCREENING

Computational screening can play an important role in discovering new materials for energy-efficient carbon capture. Carbonaceous materials, zeolites, metal-organic frameworks (MOFs), and amorphous porous carbon compounds are often considered as sorbents because of their high surface areas. The majority of membranes are polymeric. However, substantial research is being conducted on inorganic, carbonaceous, and mixed-matrix membranes (MMMs). Despite the commercial availability of amine solvents for CO_2 capture, more research is needed to establish computational frameworks capable of combining materials selection and process optimization for rapid screening of large databases of new materials for CO_2 capture with low cost and high purity and recovery. Adsorption-based carbon capture has also been the focus of several efforts to develop performance-based screening workflows.

MOFs are high-capacity CO_2 adsorbents with excellent chemical tunability in terms of pore size, pore shape, and topology, metal-site chemistry, and linker functional groups. Their sensitivity to moisture limits the applicability for CO_2 capture from flue gas laden with water vapor. In contrast, porous carbonaceous materials are both chemically and thermally stable. Typically, they are derived by the pyrolysis of a carbon-atom-containing precursor.

Porous aromatic frameworks (PAFs) are a class of porous carbonaceous materials that have capacities for CO_2 storage and separation. Although membrane technology has a smaller footprint, most membranes are unable of removing CO_2 from flue gases with high purity and recovery. MMMs can overcome this limitation by taking advantage of interactions and transfer across various composite material components and building blocks.

The complexity of composite materials provides a great opportunity for mixing and matching of materials. However, this requires an integrated experimental and computational effort. Membrane separations can be energy-efficient, but there is more scope to explore for DAC applications.

Because of their excellent physicochemical features, ionic liquids (ILs) have been suggested as a viable class of solvents for CO_2 capture. ILs have garnered a great deal of interest in the electrochemical CO_2 reduction process (CO_2RR) due to their particular benefits in reducing the overpotential and enhancing product selectivity.

Many ILs have excellent CO_2 solubilities, but their high viscosity kinetically limits the gas absorption. Encapsulation of ILs is an effective approach to overcome these limitations. Long-range Coulombic interactions may be used to adjust the structure and assembly of the molecular building blocks that impact molecular transport in either sorbent or membrane configurations in advanced ILs systems. To determine the best ILs for CO_2 capture, a computer-aided IL design (CAILD) strategy is required.

Traditional CAILD approaches for calculating gas solubility often combine an equation of state with the UNIFAC-IL model, which is computationally intensive and occasionally cannot provide satisfactory results.

PROCESS CONTROL AND SYTEM IDENTIFICATION

Dynamic modeling, system identification, and a robust process control system can make the transition easy for the integrated carbon capture processes. By doing so, the processes may operate at their best possible state, making them economically viable in the long term. Developing control strategies and operational protocols for the complex CCUS systems are challenging mainly due to its uncertain nature associated with such integrated multi-scale behavior. Using multi-scale dynamic capture models in real-time applications is also computationally intensive. As a consequence, new approaches are needed to reduce the complexity of PDE-based and rate-based dynamic models while preserving input-output characteristics. Dynamic reduced models are one of an approximation methods of high-fidelity capture models, providing a compromise between accuracy, application, and computing cost.

Nonlinear Model Predictive Control (NMPC) allows sophisticated dynamic process models for nonlinear, multivariable control with constraints, leading to online dynamic optimization satisfying economic goals. Nevertheless, economic NMPC (eNMPC) needs careful formulation of the NLP subproblem to ensure stability.

Future research will focus on creating process control frameworks intended for flexible operation and dynamic situations. Developing a deeper understanding of the process dynamics might increase the precision and robustness of dynamic process control and scheduling during flexible operation, plant start-up and shutdown, and plant start-up. On the other hand, applying strict restrictions on certain variables to minimize the gap between a value and its set-point might reduce the system’s adaptability.

While the majority of research focuses on the flexible operation of CCS capturing plant’s dynamics, comparatively few studies analyze the challenges of integrating emerging technologies when the dynamics of the processes are still not well understood. However, many other directions of the control aspects from the perspective of PSE side had been explored. For example, a BP neural network model and PID temperature control system for Capture Process by CaO Carbonation-$CaCO_3$ were built based on the modeling of the process parameters and dynamic features and they mentioned that intelligent/GA method could bring the stability, accuracy, and expeditiousness to the PID controller.

DEFINITION

Absorption – Chemical or physical take-up of molecules into the bulk of a solid or liquid, forming either a solution or compound.

Adsorption – The uptake of molecules on the surface of a solid or a liquid.

Amine – Organic chemical compound containing one or more nitrogens in -NH2, -NH or -N groups

Biomass – Matter derived recently from the biosphere.

Capture efficiency – The fraction of CO2 separated from the gas stream of a source

CBM – Coal bed methane

CCS – Carbon dioxide capture and storage.

CCUS – Carbon capture, utilization, and storage is a promising pathway to decarbonize fossil-based power and industrial sectors and is a bridging technology for a sustainable transition to a net-zero emission energy future

CDM – Clean development mechanism: a Kyoto Protocol mechanism to assist non-Annex 1 countries to contribute to the objective of the Protocol and help Annex I countries to meet their commitments.

Chemical looping combustion – A process in which combustion of a hydrocarbon fuel is split into separate oxidation and reduction reactions by using a metal oxide as an oxygen carrier between the two reactors.

Cryogenic – Pertaining to low temperatures, usually under about -100°C.

Endothermic – Concerning a chemical reaction that absorbs heat, or requires heat to drive it

EOR – Enhanced oil recovery: the recovery of oil additional to that produced naturally by fluid injection or other means.

Fischer-Tropsch – A process that transforms a gas mixture of CO and H2 into liquid hydrocarbons and water.

Flue gas - Gases produced by combustion of a fuel that are normally emitted to the atmosphere.

Fuel cell – Electrochemical device in which a fuel is oxidized in a controlled manner to produce an electric current and heat directly.

Gas turbine – A machine in which a fuel is burned with compressed air or oxygen and mechanical work is recovered by the expansion of the hot products.

Gasification – Process by which a carbon-containing solid fuel is transformed into a carbon- and hydrogen-containing gaseous fuel by reaction with air or oxygen and steam.

Geothermal - Concerning heat flowing from deep in the earth.

HHV – Higher heating value: the energy released from the combustion of a fuel that includes the latent heat of water.

IGCC – Integrated gasification combined cycle: power generation in which hydrocarbons or coal are gasified (q.v.) and the gas is used as a fuel to drive both a gas and a steam turbine

Injection – The process of using pressure to force fluids down wells

Injection well – A well in which fluids are injected rather than produced.

Ion – An atom or molecule that has acquired a charge by either gaining or losing electrons.

LHV – Lower heating value: energy released from the combustion of a fuel that excludes the latent heat of water

LNG – Liquefied natural gas

MEA – Mono-ethanolamine.

Membrane – A sheet or block of material that selectively separates the components of a fluid mixture.

NGCC – Natural gas combined cycle: natural-gas-fired power plant with gas and steam turbines

Oxidation – The loss of one or more electrons by an atom, molecule, or ion.

Oxyfuel combustion – Combustion of a fuel with pure oxygen or a mixture of oxygen, water and carbon dioxide.

Partial oxidation – The oxidation of a carbon-containing fuel under conditions that produce a large fraction of CO and hydrogen.

Partial pressure – The pressure that would be exerted by a particular gas in a mixture of gases if the other gases were not present.

Pre-combustion capture – The capture of carbon dioxide following the processing of the fuel before combustion.

PSA – Pressure swing adsorption: a method of separating gases using the physical adsorption of one gas at high pressure and releasing it at low pressure.

Reduction – The gain of one or more electrons by an atom, molecule, or ion.

Synthesis gas – A gas mixture containing a suitable proportion of CO and H2 for the synthesis of organic compounds or combustion.

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