Innovating and Commercializing Carbon Capture Processes Through Predictive Modeling

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Introduction

Carbon capture, utilization and storage (CCUS) are a crucial set of technological approaches to avoiding CO_2 emissions, directly removing CO_2 from the air and then semi-permanently removing the captured CO_2 from the ecosystem. It involves the capture of CO_2 from large point sources (such as coal or gas power generation, or industrial facilities that use either fossil fuels or biomass for process heat), or directly from air ("direct air capture"). The captured CO_2 is then compressed—unless captured adjacent to the target use site—and transported by pipeline, ship, rail or truck for use in a range of applications. It can also be used as an enhanced oil recovery (EOR) agent, where it then stays in place in the oil-bearing formation, or injected into deep geological formations, which trap the CO_2 for permanent storage.[1]

The "International Energy Agency (IEA) Energy Technology Perspective 2020" represents a commonly held viewpoint that CCUS will almost certainly play a key role in greenhouse gases (GHG) emission reduction and global energy transitions.[2] CCUS can be retrofitted to existing power and industrial plants to tackle CO_2 emissions and provide a feasible pathway and support a rapid scaling up for low-carbon, "blue" hydrogen production. It is the most effective current approach for some of the challenging emissions in heavy industries, such as cement and steel production. Carbon capture is also being demonstrated as an approach to removing carbon from the atmosphere ("direct air capture").

The 2015 Paris Agreement and the "2018 IPCC Special Report" triggered the current round of interest in carbon capture. By August 2020, 14 countries and the European Union (EU) have adopted formal net-zero emissions targets in national law or proposed legislation to that effect, with target dates of 2045, 2050 or beyond with similar targets under discussion in about 100 other countries[3]. These have led to carbon taxes across the EU, and proposed carbon taxes in many other countries and regions. Leading financial institutions and capital funding sources for industry, such as Blackrock, Barclays and JP Morgan Chase, are equally pushing this agenda. Furthermore, an alliance of capital sources, ranging from major pensions funds to major foundations (such as the Gates Foundation) and major banks, including Allianz, are pushing better carbon markets that would inject capital into carbon mitigation projects in the developing world. Recently, Bill Gates, together with leading philanthropists and innovators, launched Breakthrough Energy Ventures to push several key carbon mitigation technologies, in particular, green hydrogen and direct air capture.

The next decade will see strong development and deployment of CCUS. In the IEA's Sustainable Development Scenario, global CO_2 emissions from the energy sector could decline to net zero by 2070, and the amount of CO_2 captured would need to grow by a factor of 20 from around 40 Mt today (2020) to over 800 Mt in 2030[3], requiring a significant ramp-up in average annual additions of CO_2 capture capacity. To achieve the necessary volumes of carbon capture that carbon mitigation goals require, Dr. Robert Socolow[4], Carbon Mitigation Expert from Princeton University, estimates that over 1 billion tons of CO_2 will need to be captured and managed per year, which in pressurized liquid form is equivalent in volume to over 30 million barrels of oil that need to be transported and stored each day of the year.

One current focus of CCUS is on retrofitting existing fossil fuel-based power and industrial plants, and supporting low-carbon hydrogen production. By 2030, more than half of the CO_2 captured will be from retrofitted assets, an annual average of around 20 coal power plants will be retrofitted with capture equipment between 2025 and 2030; 18 Mt of hydrogen will be produced from CCUS-equipped facilities worldwide in 2030[3]. The second focus is on achieving effective and efficient carbon capture in purpose-built facilities, such as the current generation of "blue hydrogen" and "blue ammonia" plants, which are currently in feasibility study or design phases. For these approaches, there is new ground being covered in the innovative integration of process technologies with carbon capture and the renewable energy sources driving carbon capture.

A June 2021 survey of 186 companies across oil, chemical and related industries[5] indicates that 89 companies—or almost 50 percent of those surveyed—are today or within the next five years, planning to invest capital in carbon capture facilities. The planned application of carbon capture and ways of utilizing CO_2 show an interesting cross section, as depicted in Figure 1.

For companies contemplating integrating CO_2 capture into their assets, accurate process modeling is a crucial requirement to select the right processes and to design the most operable, energy efficient and sustainable solutions.

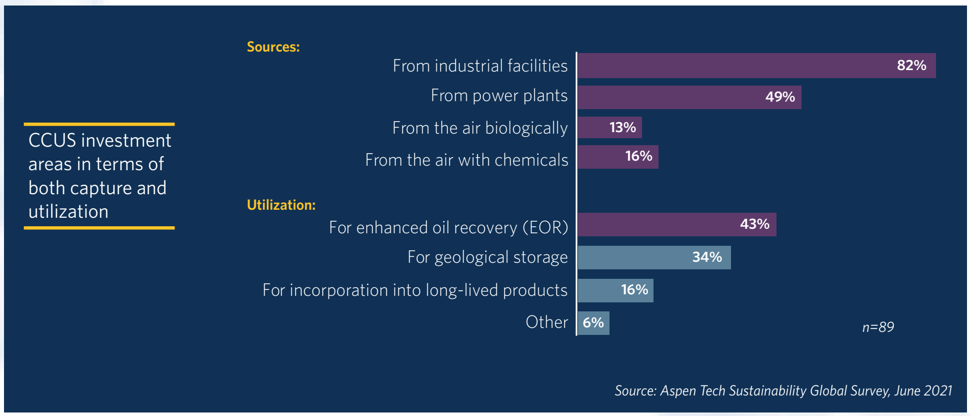

Figure 1: Carbon capture and utilization measures reported by 89 energy, chemicals, power and related companies.

Chemical and Physical Absorption Technology for CO_2 Capture

CO_2 absorption using chemical and physical solvents are the most proven processes for CO_2 capture today. Figure 2 shows a typical flow diagram for CO_2 capture by absorption. This operation is normally performed using two columns, one for CO_2 absorption and the other operating at a higher temperature, releasing the absorbed CO_2 and regenerating the solvent for further operation.

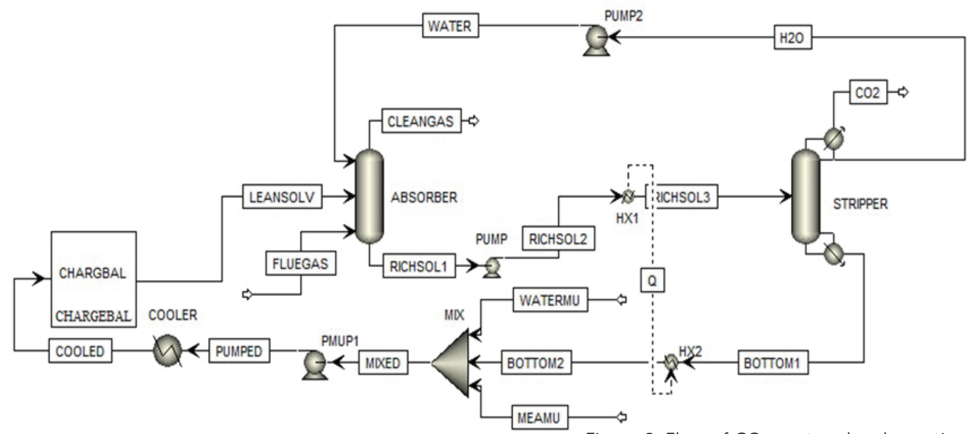

Figure 2: Flow of CO_2 capture by absorption.

CO_2 absorption by solvents is the most mature CO_2 separation technique, currently being used in power generation, natural gas processing, hydrogen production and industrial production (steel production and fertilizer plants). As of 2020, there are 21 CCUS facilities around the world with capacity to capture up to 40 Mt CO_2 each year, three more facilities under construction, and 41 facilities in early or advanced development[3]. In addition, a government-industry consortium operates a commercial-scale demonstration plant at Technology Centre Mongstad (TCM) that tests solvents, column arrangements and a membrane separation approach, and can operate on both refining unit and power generation stack flue gases.

CO_2 capture typically accounts for almost 75 percent of the cost of CCUS and can range from USD 15-25/t to more than USD 120/t[3], depending on the application and concentration of CO_2. Reducing the cost of CO_2 capture through reduced energy needs, has been the focus of research and development by private and public research centers around the world in recent years. These costs can be reduced through economies of scale, optimization of the CCUS operating conditions and supply chain, and technology development. Although capture costs have already declined substantially in the past decades, R&D will play a critical role in supporting further cost reductions to accelerate the development and deployment of CCUS.

Simulation of CO_2 Capture Processes

Process simulation software, notably Aspen Plus® and Aspen HYSYS® from AspenTech, can provide a versatile, accurate and flexible simulation environment and can be used in the process modeling, design, optimization and techno-economic evaluation for CO_2 capture.[6-9]

Property Packages for CO_2 Capture

Software such as Aspen HYSYS provides two special property packages, “Acid Gas—Chemical Solvents” and “Acid Gas—Physical Solvents,” which allow users to model CO_2 capture using chemical and physical solvents, respectively.

The thermodynamic package for the chemical solvents is based on the Electrolyte Non-Random Two-Liquid (Electrolyte NRTL) model for electrolyte thermodynamics and Peng-Robinson Equation of State for vapor phase properties. It includes all the necessary aqueous-phase equilibrium and kinetics reactions required for rigorous calculations of the process.

The package for the physical solvents is based on two equations of state: the Perturbed Chain Statistical Association Fluid Theory (PC-SAFT) equation of state for Dimethyl Ether of Polyethylene Glycol (DEPG), a constituent of a commercially available solvent called Selexol®, and the Cubic Plus Association (CPA) equation of state for methanol.

Regression and validation have been performed with available VLE and heat of absorption data for many solvents, including all major solvents used in the industry, such as MEA, MDEA, DEA, PZ+MDEA, DGA, DIPA, Sulfolane-DIPA, Sulfolane-MDEA, TEA, DEPG and methanol.

The validation results for CO_2 solubilities in the aqueous MEA solution and DEPG are shown in Figures 4 and 5. The regressed and validated parameters are stored in the proprietary Acidgas databank. When the Acidgas fluid package

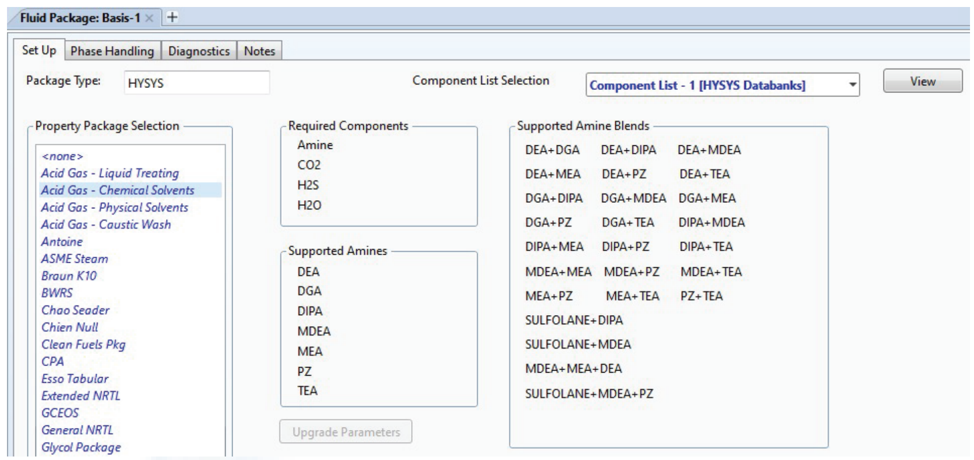

Figure 3: Fluid packages for CO_2 capture in Aspen HYSYS.

is selected within HYSYS, the parameters in the databank can be used in the calculation automatically.

Aspen Plus supports all of the same thermodynamic models (Electrolyte NRTL, PC-SAFT and CPA) and the Acidgas databank for CO_2 capture. Furthermore, Aspen Plus includes several model templates with all relevant pure component parameters, binary parameters and reaction parameters to model the chemical and physical solvent-based capture processes. Additionally, Aspen Plus allows users to utilize their own parameters for the property models, which offers more flexibility in specifying and evaluating new solvents and other adsorption approaches (such as the zeolite approach being pursued by Carbon Capture Inc).

Rate-Based Distillation

Aspen Plus and Aspen HYSYS support two approaches to model distillation columns: rate-based and equilibrium-stage. The equilibrium approach is the most common modeling approach, and is more accessible to a wider population of modeling users. However, the rate-based approach is more accurate and has proven to be particularly valuable to accurately predict performance of carbon capture.

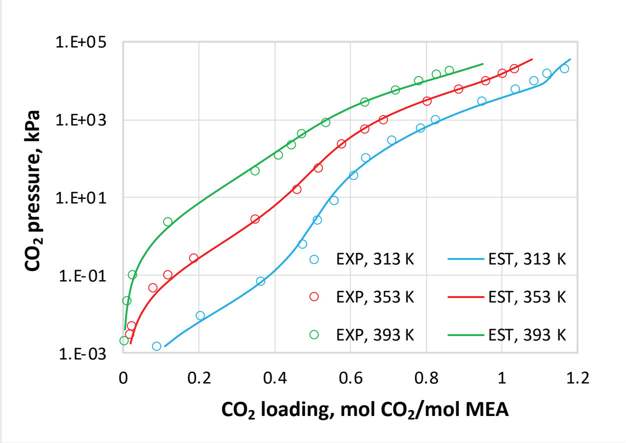

Figure 4: Experimental data from Jou, et.al. (points) compared to model prediction: (lines).[10]

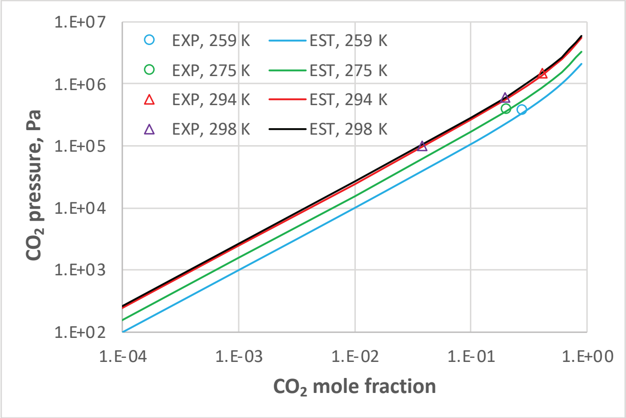

Figure 5: Experimental data from Kutsher, et.al. (points) compared to model prediction: (lines).[11]

Rate-based models utilize mass and heat-transfer correlations based on transfer properties and tray/packing geometry, assuming that separation is limited by mass transfer between the contacting phases. This makes them more accurate over a wider range of operating conditions, as the equilibrium-stage models require empirical adjustments for accurate simulation.[12]

Rate-based technology is the most reliable way to model columns with reaction and to design columns without having information about tray efficiencies or HETP (height equivalent to a theoretical plate) for packed columns. Implementing rate-based modeling allows users to simulate actual column performance more closely, enabling them to make more accurate predictions over a wider range of operating conditions with less fitting of data. This is particularly useful for CO_2 absorption processes, where component efficiencies vary widely. Rate-based modeling allows users to extrapolate outside current operating ranges with more confidence, which is advantageous when limited data is available. This in turn allows users to produce tighter designs with confidence, leading to designs that are optimized for energy consumption, and capital and operating costs.[12]

Table 1: Validation of pilot plant data.[13]

Case	PCO_2, mbar	Lean loading	Rich loading		CO_2 removal, %		Energy, MJ/kgCO_2	
	Exp	Exp	Exp	Sim	Exp	Sim	Exp	Sim
A1	54	0.041	0.45	0.475	81	80	10.3	11.5
A2	54	0.13	0.448	0.470	91	94	3.72	4.95
A3	54	0.205	0.465	0.467	91	88	3.76	3.88
A4	54	0.259	0.438	0.444	91	91	4.2	4.02
A5	54	0.25	0.388	0.399	90	89	4.72	4.80
A6	54	0.276	0.415	0.417	90	90	4.63	4.27
A7	102	0.087	0.52	0.484	87	84	6.37	6.03
A8	102	0.131	0.507	0.477	90	90	4.65	4.55
A9	102	0.205	0.464	0.467	90	90	4.07	3.97
A10	102	0.186	0.437	0.454	91	95	4.09	4.17
A11	102	0.212	0.444	0.442	87	94	4.22	4.27
A12	102	0.23	0.427	0.422	91	93	4.56	4.39
A13	102	0.23	0.515	0.485	93	87	3.63	3.86
A14	102	0.208	0.481	0.478	91	91	3.82	3.78
A15	54	0.222	0.511	0.477	88	82	3.23	3.84
A16	54	0.204	0.494	0.471	91	89	3.57	3.91
A17	54	0.203	0.494	0.466	90	85	3.88	3.97
A18	102	0.308	0.479	0.483	58	62	3.95	3.90
A19	102	0.233	0.461	0.477	78	72	3.94	3.88
Absolute average relative error, %				3.3		3.3		6.3

In addition to validating the thermodynamic model with physical properties data, the simulation model has also been validated against pilot plant data as seen in Table 1.

Column Hydraulic Analysis

Recent versions of Aspen Plus and Aspen HYSYS provide column hydraulic analysis features, enabling semi-automated column sizing, performance rating and visualization of hydraulic operability and hydraulic constraints.

Understanding column hydraulics is an important aspect of column design. The trays and packings within a column can put limits on the operation of the process. Outside that range, problems like weeping, jet flood and downcomer backup can occur. By fully understanding the column mechanisms, users can address columns with limited capacity, high energy costs and product quality issues.

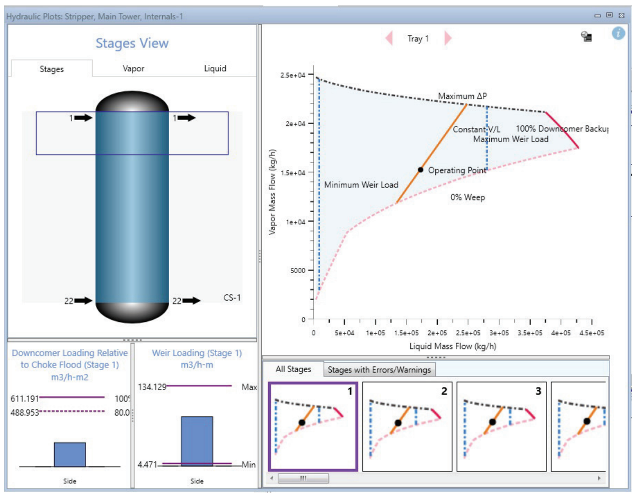

Figure 6: Hydraulic plots in Aspen HYSYS.

Column analysis can be used for many different tasks. In new design and revamps, engineers can use it to maximize capacity and minimize operating costs by optimizing column performance, reuse equipment in revamps to minimize capital expenses, and maximize operability ranges through operating conditions evaluation, maintaining safe operations and avoiding operational issues.

Process models can be put online as digital twins to optimize production, reduce operating costs, increase asset utilization, diagnose operating issues and quickly evaluate process changes to return to normal operation.

Greenhouse Gas Emissions

It's easy for process engineers to estimate greenhouse gas emissions associated with a process within Aspen Plus and Aspen HYSYS. The greenhouse gas emissions are reported in terms of CO_2 equivalents of global warming potential (GWP). The carbon equivalents of streams are based on data from three popular standards for reporting such emissions: the IPCC's 2nd (SAR) and 4th (AR4) Assessment Reports, and the U.S. EPA's proposed rules from 2009.

Two sources of GHG emissions are considered: the direct generation of greenhouse gases within the process (also known as "Scope 1" emissions); and indirect generation of GHG resulting from process utilities, including heating and cooling (also known as "Scope 2" emissions). In addition, users can specify the carbon fee or tax and estimate the associated carbon emissions costs.

Ultimately, these features make it easy for the user to evaluate the "carbon equivalents" generated by the process and make more informed design decisions.

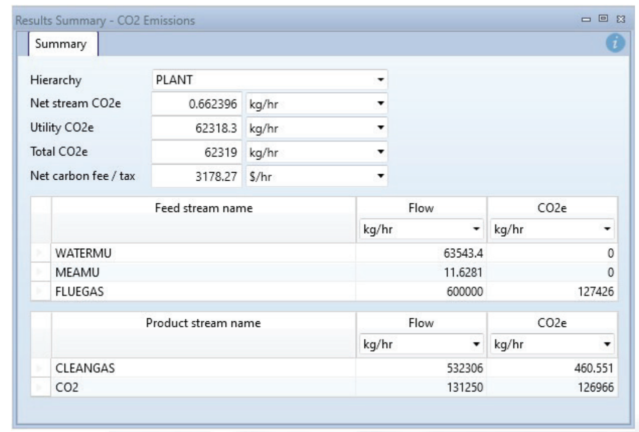

Figure 7: CO_2 emissions report in Aspen Plus.

Activated Economic Analysis

Users can easily estimate costs with Aspen Plus and Aspen HYSYS through Activated Economic Analysis. This integrated feature within the simulator allows cost estimation based on the process simulation results and optimization of capital and utility costs for plant designs.

Once users obtain simulation/process data for streams and unit operations, they can set up the model for economic analysis by identifying any process stream and process utility conditions, map the unit operations to constituent equipment, and then size and customize the equipment based on standards and process needs. Next, the cost of the process can be evaluated based on the sizing, and an analysis of the reported cost and investment metrics can be used to optimize the process or make it more cost efficient.

When process engineers work with estimators, estimators can further tune the economic models. Through this tuning process, estimators can calibrate the built-in cost models to reflect a given company's cost bases, procurement agreements and regional benchmarks to increase accuracy of the techno-economic analysis. For the rapidly maturing technology area of CO_2 capture, this combined process/economic modeling approach is crucial to capital planning and investment decisions and is a highly differentiated aspect of the AspenTech modeling solution.

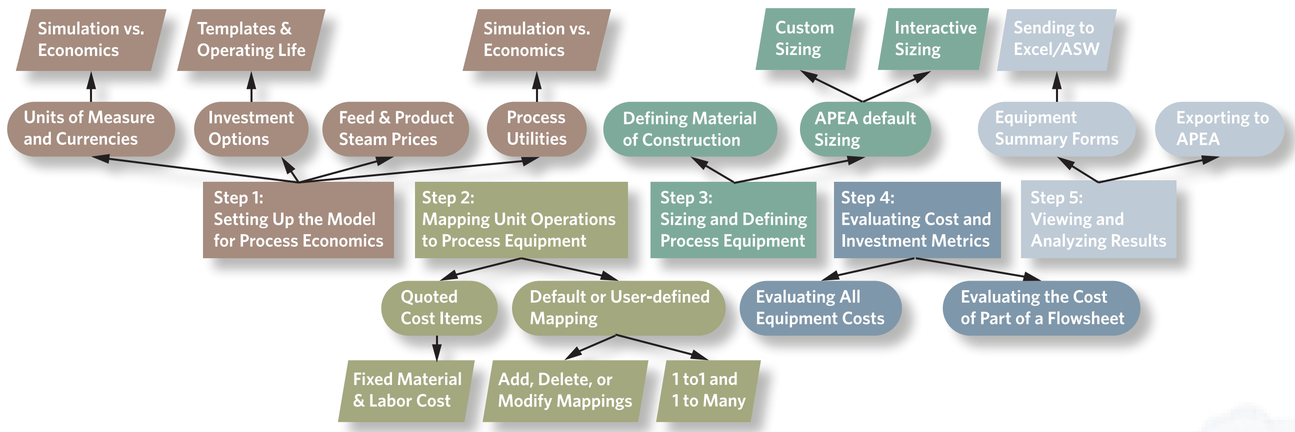

Figure 8: Workflow for economic analysis.

Other Emerging Carbon Capture Approaches

Other technology approaches beyond solvent absorption are currently being developed for carbon capture. These include membrane separation approaches and other novel methods. Many of these approaches are proprietary at this time and are beyond the scope of this white paper. A number of technology start-ups pursuing these approaches are employing the AspenTech platforms to simulate and predict the performance of these novel methods.

Conclusion

CCUS can play an important and diverse role in meeting global energy and climate goals. A rapid scale-up of CCUS deployment is needed with a focus on the retrofitting of power plants and supporting low-carbon hydrogen production into the next decade. CO_2 absorption using chemical and physical solvents is a mature CO_2 capture technique and can be applied to power generation and hydrogen production to tackle CO_2 emissions. Even though capture costs have already declined significantly in the past decades, it's still necessary to reduce the costs for the acceleration of CCUS deployment.

Users can utilize Aspen Plus and Aspen HYSYS with the integrated features (e.g., Column Analysis, CO_2 emissions and Economic Analysis) for process simulation and equipment design, process optimization and cost reduction. Aspen Plus and Aspen HYSYS provide special property packages and more accurate rate-based modeling of CO_2 capture. The Column Analysis feature supports distillation column sizing and rating while Economic Analysis can estimate the capital and operating costs. Finally, CO_2 emissions can also be reported within Aspen Plus and Aspen HYSYS. New example models for industrial-scale CO_2 capture have been released in V12.1, and eLearning courses and webinars will be available in the near future.

Citations

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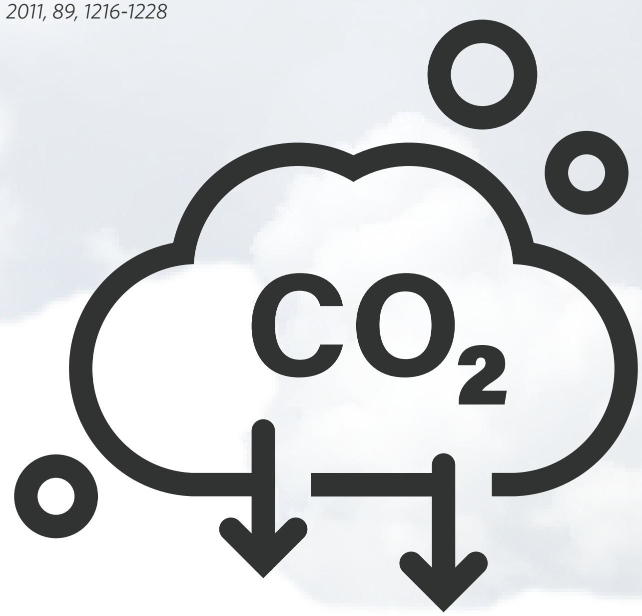

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