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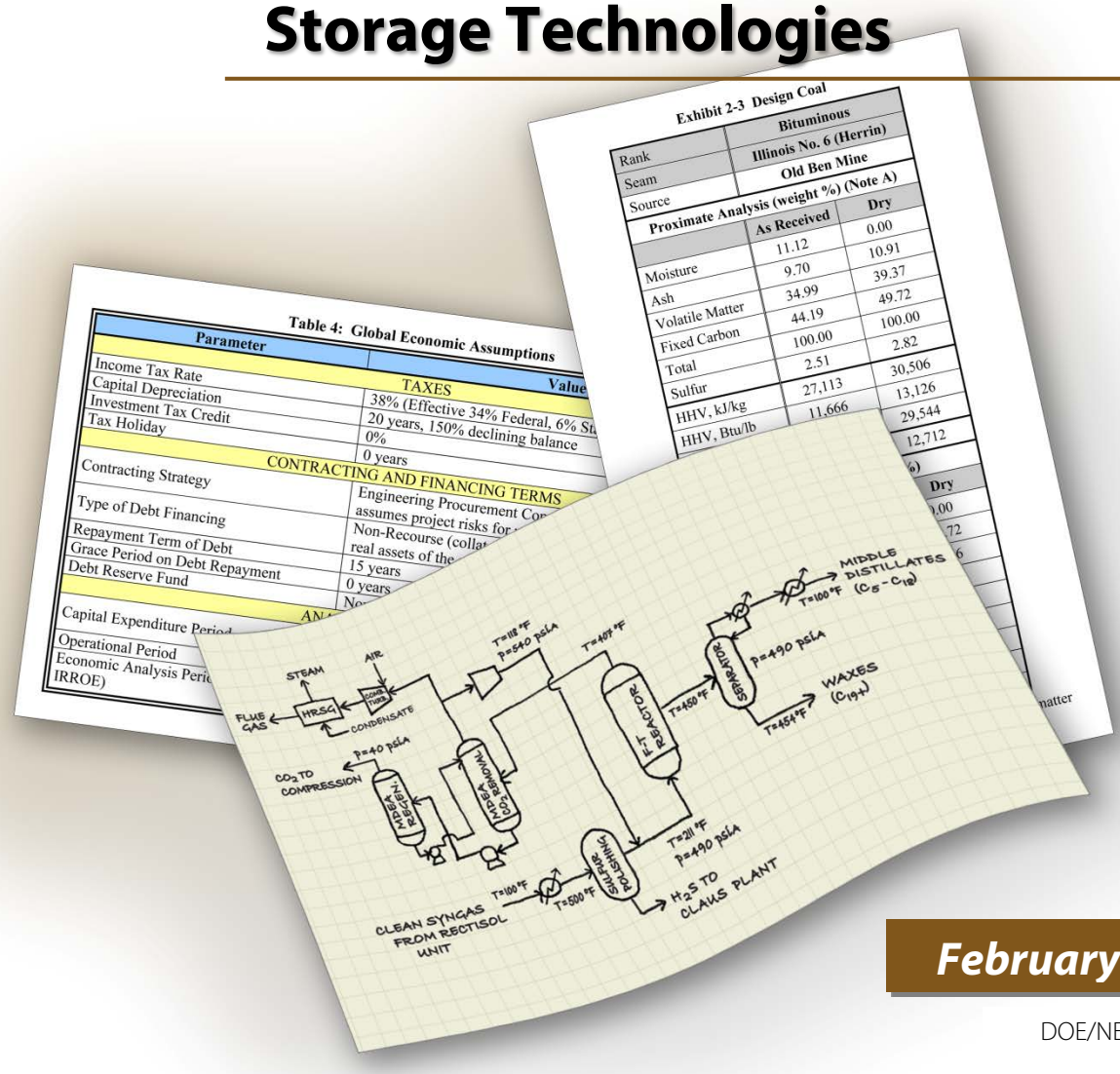
QUALITY GUIDELINES FOR ENERGY SYSTEM STUDIES

Cost and Performance Metrics Used to Assess Carbon Utilization and Storage Technologies



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Final Report

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NETL Contact:

Gregory Hackett
General Engineer
Office of Program Performance & Benefits, Performance Division

National Energy Technology Laboratory
www.netl.doe.gov

Prepared by:

Energy Sector Planning and Analysis (ESPA)

Peter Kabatek
WorleyParsons Group, Inc.

Alexander Zoelle
Booz Allen Hamilton, Inc.

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Acronyms and Abbreviations

CCUS	Carbon capture, utilization, and storage	NETL	National Energy Technology Laboratory
CO_2	Carbon dioxide	NFPA	National Fire Protection Association
DOE	Department of Energy	R&D	Research and development
ESPA	Energy Sector Planning and Analysis	t	tonne (1,000 kg)
h, hr	Hour	U.S.	United States

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1 Background

In an effort to reduce carbon dioxide (CO_2) emissions from various industrial and power generation processes to the atmosphere, the United States (U.S.) Department of Energy (DOE) National Energy Technology Laboratory (NETL) is funding research intended to advance state-of-the-art technologies that address the use of CO_2 in a variety of processes. Much of this research is funded and managed in the CO_2 Utilization Focus Area of the Carbon Storage Program. [1]

CO_2 utilization efforts focus on pathways and novel approaches for reducing CO_2 emissions by developing beneficial uses for CO_2 that will mitigate greenhouse gas emissions. Utilization is an important component in carbon sequestration, also called storage. Some of the applicable approaches are conversion of CO_2 into useful chemicals and polycarbonate plastics, storage of CO_2 in solid materials having economic value, indirect storage of CO_2, and other breakthrough concepts. The term sequestration for this report is defined as the segregation of CO_2, either chemically, as in chemical utilization, or physically, as in geologic storage. This concept is therefore named carbon capture, utilization, and storage (CCUS).

Critical challenges identified in the utilization focus area include the cost-effective use of CO_2 as a feedstock for chemical synthesis, or its integration into pre-existing products. The efficiency (reaction conversion and the amount of CO_2 sequestered in a product) and energy use (the amount of energy required to utilize CO_2 in existing products) of these utilization processes also represent a critical challenge.

In order to meet these challenges, metrics are developed to enable comparison of such technologies and utilization processes. In the not-too-distant past, authors and organizations have described using "sustainability metrics" to guide decision-making in the process industries for the goals of environmental protection, economic prosperity, and social benefit. [2, 3, 4, 5]

2 Introduction

A *metric*, in the context we are using here, is defined as "a standard of measurement." [6]

Various aspects of research and development (R&D) projects, also thought of as processes or technologies, can have standards of measurement developed and defined for them. The purpose of this section of the Quality Guidelines is to provide a methodology for developing these standards of measurement.

The two most common groups of metrics are those dealing with economics (costs and values of inputs, outputs, and processes, including capital and operating costs) and performance (mass conversion, energy efficiency, and, generally speaking, energy and mass balance derived parameters).

Economic and performance metrics are needed to be able to compare and/or screen varied R&D projects and technologies from different perspectives or points of view. It is important to have available as wide a set of metrics as possible, because, at this stage of development, there are usually gaps in the information available; these vary from project to project and technology to technology, such that not every metric can be evaluated for each. Having a diverse set of metrics

allows for R&D projects and technologies to be compared by at least one or more of these metric methods, and for meaningful comparisons to be drawn.

Depending on the priorities of an organization or the goals of R&D programs, different metrics may be weighted differently in their application. Thus, some metrics may be considered more important than others.

Such assessments and comparisons assist in decision-making for allocating limited funds and resources to the most promising processes or technologies, according to the metrics which are judged to be the most important.

The metrics developed here are applied to CO_2 utilization for beneficial use. This utilization of CO_2 involves the chemical conversion of the CO_2 into useful and valued products (such as polycarbonate plastics), or integrating the CO_2 into pre-existing products (such as cement or concrete).

3 Developing the Metrics

When developing the metrics for the utilization of CO_2, it is important to understand the essence of the utilization technology or process, as well as to ask the following questions:

- What reactions are involved?
- What are the reactants and co-reactants?
- What are the products and co-products?
- What are the reaction conditions?
- What are the heats of reaction?
- What catalysts and co-catalysts are required?
- Where are the system boundaries drawn?
- Is the system batch, or continuous and steady-state?
- At what scale has the technology or process been demonstrated?

In cases where the new CO_2 utilization technology or process, also referred to as pathway, has a corresponding existing or traditional non-utilization pathway for the product of interest, it is important to understand all the pertinent details of that pathway, because some of the metrics compare the new pathway benefits relative to the traditional one.

It is useful to consider various aspects of each technology or process under each of the categories of economics and performance.

Questions to be asked under economics are as follows:

- What market does the process product target, and what is the size of the market?
- What are the unit and total costs of all the material (feedstocks) and energy inputs at the conditions required by the reaction(s), or at the system boundary?
- What is the availability of all material feedstocks required?

- What are per unit and total costs (or values) of all the material and energy outputs, including any waste streams, as they exit the reaction, or as defined at the system boundary?
- What are the capital costs of all the equipment specified within the system boundary?
- What are operating costs of the process as specified within the system boundary?
- What is the reactor volume required for the scale of the process?
- What is the plot space required for the scale of the process?
- What are the known hazards, and what are the likely safeguards?
- If the new process is replacing an existing process, what are the above parameters for the existing process?

Questions to be asked under performance are as follows:

- What is the conversion efficiency or yield of each reaction at the specified reaction conditions?
- What is the mass and energy balance, including pressures, temperatures, flowrates, compositions, and process flow diagram, for the system as defined above?
- Has the technology or process been demonstrated as a working system, including any recycle streams, heat integration, and intermediate and/or final separation of products to meet specified product purities?
- What is the consumption rate and useful life of any catalysts/co-catalysts?
- What is the intermittent or continuous rate of any purge or waste streams and are these streams hazardous materials?
- If the new process is replacing an existing process, what are the above parameters for the existing process?

4 Methodology

The methodology for 12 metrics that were developed for CO_2 utilization technologies and processes is detailed below. The 12 metrics are grouped under the following five subheadings:

- Performance
- Cost
- Emissions
- Market
- Safety

4.1 Performance Metrics

4.1.1 CO_2 Utilization Efficiency

CO_2 utilization efficiency is defined as the amount of CO_2 utilized (mass basis) per unit amount of CO_2 fed to the utilization process. This represents the simplest way of thinking about a CO_2 utilization metric. It is a dimensionless ratio and is preferably expressed as a percentage. The higher the percentage, the more efficient the CO_2 utilization process.

For a continuous flow process, this metric is expressed as the flow rate of CO_2 into the process minus the flow rate of CO_2 leaving the process divided by the flow rate of CO_2 into the process.

$$CO_2 \text{ Utilization Efficiency (\%)} = \frac{\text{tonnes } CO_2 \text{ utilized}}{\text{tonnes } CO_2 \text{ fed to process}} \times 100$$

$$= \frac{(\text{tonnes/year } CO_2 \text{ in - tonnes/year } CO_2 \text{ out})}{\text{tonnes/year } CO_2 \text{ in}} \times 100 \qquad (1)$$

4.1.2 CO_2 Utilization Potential

CO_2 utilization potential is the amount of CO_2 that would be utilized (mass basis) to meet the desired product's market demand, relative to the amount of CO_2 emitted from a user-specified reference CO_2 emitter or plant. This metric represents the CO_2 emission stream's potential to be utilized in a marketable product. It is a dimensionless ratio and can be expressed as a percentage. The geographic basis for the product market demand should be specified, e.g., the U.S., North America, or the world. Also, the CO_2 emission stream reference basis should be defined, since the metric is dependent on this reference, e.g., a single power plant emission, total U.S. coal-fired power plants emissions, etc. Furthermore, the reference CO_2 basis can be further defined as the CO_2 emitted, or as the CO_2 captured in a carbon capture scenario. In the latter definition, the CO_2 captured represents the CO_2 available to the utilization process.

$$CO_2 \text{ Utilization Potential (\%)} = \frac{\begin{array}{c}\text{tonnes/year } CO_2 \text{ utilized} \\ \text{to meet market demand}\end{array}}{\begin{array}{c}\text{tonnes/year } CO_2 \text{ available} \\ \text{from reference plant}\end{array}} \times 100 \qquad (2)$$

4.1.3 CO_2 Utilization Intensity

CO_2 utilization intensity is the amount of CO_2 utilized (mass basis) per unit amount of the desired product. This metric is a dimensionless ratio and should be expressed as a percentage. It may be thought of as a 'mass version' of the chemical reaction stoichiometry (which is done on a mole basis).

$$CO_2\ Utilization\ Intensity = \frac{tonnes\ CO_2\ utilized}{tonnes\ product\ produced} \times 100$$

$$= \frac{(tonnes/year\ CO_2\ in - tonnes/year\ CO_2\ out)}{tonnes\ product\ produced} \times 100 \quad (3)$$

4.1.4 CO_2 Integration Reaction Rate

The CO_2 integration reaction rate is the molar rate of CO_2 utilized per unit of reactor volume. The molar rate can be on any time basis, such as lb-mol/hr, and the reactor volume can be on any convenient volume basis, such as gallons. In this case, the metric units would be lb-mol/(gal·hr). This metric is a measure of the reactor volume required in the technology's current state of development to meet the desired production rate.

$$CO_2\ Integration\ Reaction\ Rate\ (lb\text{-}mol/gal \cdot hr) = \frac{lb\text{-}mol/hr\ CO_2\ utilized}{gallons\ of\ reactor\ volume\ required\ for\ reaction} \quad (4)$$

4.1.5 CO_2 Energy Utilization

The CO_2 energy utilization metric is defined as the net amount of energy required per unit amount of CO_2 utilized (mass basis). It is a measure of the energy efficiency of the technology or process to utilize CO_2. The units for the energy utilization metric are kW/(tonne CO_2 per hour).

$$CO_2\ Energy\ Utilization\ (kW/(tonne\ CO_2/hr)) = \frac{kW\ energy\ required}{tonnes/hour\ CO_2\ utilized} \quad (5)$$

4.2 Cost Metrics

4.2.1 Product Marketability

The product marketability metric is the cost to make a unit amount of the desired product relative to the market value of that product. This metric is a dimensionless ratio and should be expressed as a percentage.

$$Product\ Marketability\ (\%) = \frac{\$\ cost\ to\ make\ a\ tonne\ of\ desired\ product}{\$\ per\ tonne\ market\ value\ of\ desired\ product} \times 100 \quad (6)$$

4.2.2 Incremental Cost Reduction

If there is a traditional process for making the desired product that the new CO_2 utilization process is replacing, then the incremental cost reduction metric is the incremental reduction in cost by the new utilization process over the traditional process. The units of this metric are $ per tonne of product. This metric needs to have a positive value to show there is a cost saving to be had in replacing the traditional process.

$$\text{Incremental Cost Reduction (\$/tonne)} = \text{(\$ cost to make a tonne of product by traditional process) - (\$ cost to make a tonne of product by new process)} \quad (7)$$

4.2.3 Cost per Tonne CO_2 Utilized

The cost per tonne of CO_2 utilized metric is the sum of annualized capital and operating costs of the utilization process relative to the tonnes of CO_2 utilized. The costs of the process are to include infrastructure, raw materials, processing, byproduct disposal, and utilities costs, as well as any other costs. The units of this metric are $ per tonne of CO_2. This metric is dependent on the maturity or stage of development of the technology or process, and whether the costs are known or can be reasonably estimated.

$$\text{Cost per Tonne } CO_2 \text{ Utilized (\$/tonne)} = \frac{\sum \text{[annualized capital and operating costs, \$/year]}}{\text{tonnes/year } CO_2 \text{ utilized}} \quad (8)$$

4.3 Emissions Metrics

4.3.1 CO_2 Emissions Reduction

If there is a traditional process for making the desired product that the new CO_2 utilization process is replacing, then the CO_2 emissions reduction metric is the amount of CO_2 emissions reduction per unit amount of product in the new process, relative to that in the traditional process. This metric is a dimensionless ratio and should be expressed as a percentage. The greater the value, the greater is the CO_2 emissions reduction.

$$CO_2 \text{ Emission Reduction (\%)} = \frac{\text{tonnes/year } CO_2 \text{ emitted in existing process} - \text{tonnes/year } CO_2 \text{ emitted in new process}}{\text{tonnes/year } CO_2 \text{ emitted in existing process}} \times 100 \quad (9)$$

4.3.2 CO_2 Avoided Potential

If there is a traditional process for making the desired product that the new CO_2 utilization process is replacing, then the CO_2 avoided potential metric is the amount of CO_2 avoided by the new process over the traditional process, and assumed to offset CO_2 emissions from a user-specified reference CO_2 emitter or plant. This metric is a dimensionless ratio and should be expressed as a percentage. Put another way, the CO_2 avoided potential is the percentage of the reference plant CO_2 emissions that the new process would avoid producing, when considering the utilization process and reference CO_2 emitter within the same envelope.

$$CO_2 \text{ Avoided Potential (\%)} = \frac{\text{tonnes/year of } CO_2 \text{ avoided to meet market demand}}{\text{tonnes/year of } CO_2 \text{ emitted from reference plant}} \times 100$$

$$= \frac{\text{tonnes/year } CO_2 \text{ emitted from existing process - tonnes/year } CO_2 \text{ emitted from new process}}{\text{tonnes/year of } CO_2 \text{ emitted from reference plant}} \times 100 \quad (10)$$

4.4 Market Metric

4.4.1 Product Supply-Demand

The product supply-demand metric is the percentage of the desired product market that can be satisfied with the new process or technology, taking into consideration feedstock or catalyst availability, or other limitations. This metric is a dimensionless ratio that should be expressed as a percentage. The geographic basis for the product market demand should be specified, e.g., the U.S., North America, or the world.

$$\text{Product Supply-Demand Metric (\%)} = \frac{\text{tonnes/year of product that can be produced}}{\text{tonnes/year of market demand for that product}} \times 100 \quad (11)$$

4.5 Safety Metric

4.5.1 Relative Safety and Environmental Benefits

The relative safety and environmental benefits metric is a composite assessment of the raw materials and processing conditions, including any environmental benefits, of the new process relative to those of any existing process for the same product. The metric assessment is either improved, no change, or reduced.

The relative safety ranking uses the National Fire Protection Association (NFPA) Standard 704 “fire diamond” category hazard values, which range from 0 to 4, with 0 meaning no hazard and 4 meaning severe hazard. [7] The NFPA categories are those of health, flammability, and instability/reactivity. There is also a special notice category for oxidizing materials, materials having unusual reactivity with water, and simple asphyxiants. [8]

An improved relative safety assessment could be based on reduced reactor temperature and/or pressure, elimination of a hazardous feedstock or catalyst, etc.

Examples of improved environmental benefits assessments include the elimination of a petroleum-based feedstock, elimination of a toxic by-product, reduction in raw water consumption, or reduction in air pollutant emissions.

5 Conclusions

The metrics presented in this quality guideline were developed for use with CO_2 utilization through chemical conversion processes. Other types of metrics could be developed as desired, such as those used for chemistry: yield, atom economy, and reaction mass efficiency. [4]

These metrics give simple standards of measurement to gauge performance and economics of R&D projects relative to their contemporary counterparts, and between interdisciplinary utilization fields. This in itself provides useful tools for decision-makers for benchmarking performance, tracking improvement, evaluating products and processes, and developing strategies for prioritizing and allocating limited resources, such as R&D funding. [3]

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