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Designing for the Future: The Role of Process Design in Decarbonization and Energy Transition

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INTRODUCTION

The overarching goal of process design (Figure 1) is to find technologically feasible, operable, economically attractive, safe and sustainable processing pathways and process configurations with specifications for the connectivity and design of unit operations that perform a set of tasks using selected functional materials (e.g., catalysts, solvents, sorbents, etc.) to convert a set of feedstocks or raw materials into a set of products with desired quality at a scale that satisfies the demand. Process synthesis and integration can further screen, optimize and improve these pathways for given techno-econo-environmental targets or objectives. These objectives may include, but are not limited to, minimizing the overall investment and processing costs, minimizing the energy consumption, minimizing the emissions or wastes, maximizing the profit, and enhancing the safety, operability, controllability, flexibility, circularity, and sustainability, among others.

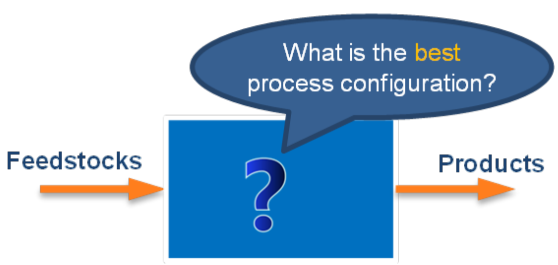

Figure 1. Overarching goal of optimal process design.

For a long time, fossil fuels (petroleum, natural gas, and coal) have been predominantly used as primary feedstocks as well as primary energy providers for the chemical process industry (CPI). The chemicals and refining is by far the largest contributor of industrial direct and indirect carbon emissions [1]. In recent times, decarbonization and transition to renewable energy have emerged as the major pathways for reducing anthropogenic greenhouse gas emissions that contribute to global warming and climate change. Like many other sectors, CPI is considering them to reduce its overall carbon footprint.

Industrial decarbonization primarily refers to reduction or elimination of CO_2 emissions from a manufacturing process. For CPI, it would include the following, among others [1]: (i) improving energy efficiency through novel process design, optimization and integration, (ii) incorporating bridging reduced/net-zero/negative emission technologies such as carbon capture, utilization and storage (CCUS) [2], direct air capture (DAC), hydrogen and/or biomass based energy & fuels, (iii) electrification of process heating and cooling, and (iv) substitution of fuels, feedstocks, and energy sources.

Energy transition is another broad concept that encapsulates a significant shift in the way we produce, distribute, and use our primary energy sources. Typically, it refers to move from conventional fossil fuels to more sustainable and environmentally friendly alternatives, such as renewables (solar, wind, hydro, geothermal), energy storage technologies, and increased energy efficiency measures.

This work explores the pivotal role of process design and optimization as the CPI navigates through different challenges and opportunities towards mitigating carbon emissions and facilitating the shift towards renewable energy.

CHALLENGES AND OPPORTUNITIES

While these measures show great promise for reducing carbon emissions, an effective integration and deployment of these measures pose are significant and, in some cases, unique challenges for the CPI. Chemical and refining processes are historically developed considering a steady supply of conventional feedstocks and energy. High efficiency and low capital intensity, both of which contributed to high economic gain, were achieved through economies-of-scale of large, centralized processing facilities. However, as we consider shifting towards utilizing unconventional feedstocks and renewable energy sources, we loose the economies-of-scale. Many unconventional feedstocks and most renewable energy sources are distributed, only intermittently available, and uncertain. One such example is shown in Figure 2, where we observe significant variability in the long-term, seasonal, and daily availability of methane from landfill gas, which is an unconventional feedstock.

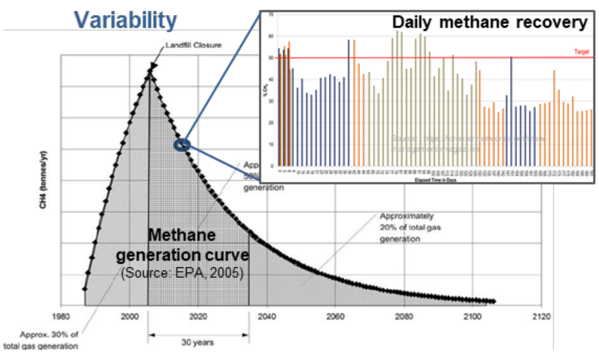

Figure 2. Long-term, seasonal and daily variability in landfill-based methane feedstcok availability.

Similar to the unconventional feedstocks, renewable energy sources such as solar and wind are distributed and intermittent. The future price of renewable electricity could decrease substantially to compete with traditional fossil fuels [3]. However, intermittency, spatio-temporal variability and non-dispatchability of renewables pose considerable challenges for systems integration. Figure 3 shows an example of variability of solar and wind energy availability.

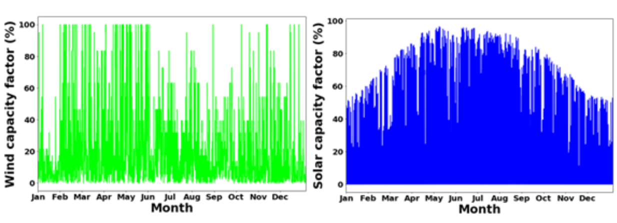

Figure 3. Temporal variability in solar and wind energy.

The intermittency of these variable renewable sources and the high energy requirement of carbon capture restrict their widespread deployment in the CPI. This often leads to simultaneous design and scheduling problems [4]. These challenges are traditionally addressed independently at the grid-level, leading to conservative costs and limited operational flexibility for both systems. However, opportunities exist to examine the synergistic integration of renewables and flexible carbon capture with individual chemical plants. Renewables can provide clean energy for carbon capture, while energy storage can be incorporated to counter renewable intermittency. To assess whether the benefits obtained from integration outweigh the capital cost under spatiotemporal variability of electricity markets and renewable energy, we can develop and use mathematical programming-based optimization frameworks for process design and optimization. We can decouple the design and operational decisions in a two-stage optimization strategy to efficiently solve the large-scale problem.

Electrification of the chemical industry reduces the reliance on fossil fuels across the economy and enables plants to integrate cleaner energy sources such as renewables. However, the variation and intermittency in renewable energy supply is a key challenge in electrifying industrial processes. Plant-wide energy storage will most likely play an important role in electrification by leveling off the change in energy supply [5]. Thermal energy storage (TES) is particularly suitable for chemical process plants due to the use of low-cost storage mediums. With the support from TES, renewable powered electric heaters can be introduced. However, there is a need for systematic methods that simultaneously consider the time-varying utility supply from renewables, the design and integration of single/multistage TES process configurations with heat exchanger networks, the scheduling of optimal charging/discharging operations, and the selection of energy storage mediums. One such concept of renewable-powered electrification is illustrated in Figure 4.

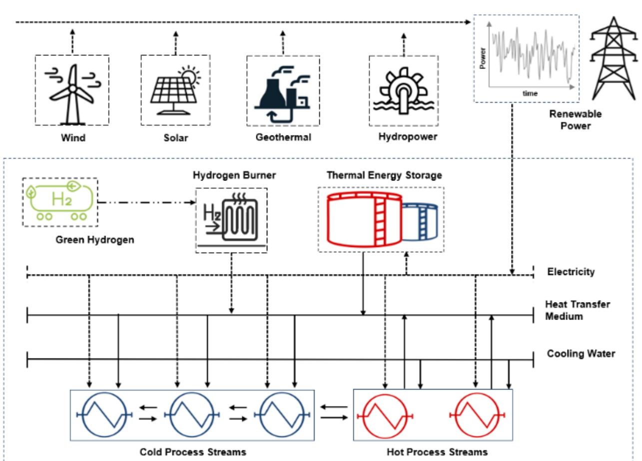

Figure 4. Renewable powered chemical process heat integration with TES and backup green hydrogen.

By integrating advanced modeling techniques, simulation tools, and artificial intelligence, engineers can further optimize the performance of existing processes and develop novel, sustainable solutions under uncertainty.

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