**Sustainable Mitigation of Carbon Dioxide to Chemicals**

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**Introduction**

The industrial processes exert significant impact on our society, economy, and environment. During the process of converting natural resources into useful products, pollutants are often discharged into our atmosphere. The pollutants have adverse effects on the society’s health, environment, and opportunities for future generations. Designing a chemical process has to address the three primary challenges: society, profit and environment. A process design that satisfies the triangle without compromising process safety is often known as sustainable design. A multidisciplinary approach known as process integration is employed to achieve sustainable design. This module addresses the use of process integration in optimizing sustainable carbon dioxide mitigation processes.

The educational module focuses on using process integration to create a superstructure of carbon dioxide transformation processes to produce profitable products. This will be followed by optimizing the superstructure to identify the most promising processing routes that result in maximum profit and carbon dioxide fixture. Students will have to balance these competing aspects as part of the module activities included.

The module consists of a series of activities that guide the students to stepwise sustainable process design. Students will begin by researching literature for synthetic routes that utilizes carbon dioxide as a reactant to form profitable products. Afterwards, students will be prompted to formulate objective function to maximize profit generated by different processes subject to given constraints dictated by the corresponding processing route. Finally, the students will use optimization software LINGO to solve for the technologies that maximizes profit.

**Rationale: Combating global warming by sustainable Carbon dioxide mitigation**

Carbon dioxide is one of the most abundant greenhouse gases emitted in excess as a result of many chemical processes. The chemistry of carbon dioxide molecule allows solar radiation to pass through earth’s atmosphere, but does not permit heat to make a journey back to space (Al Bredenberg 2012). Instead, carbon dioxide trapped in the upper layers of the atmosphere re-radiates the thermal energy back to earth’s surface increasing the atmosphere’s temperature. While moderate amount of greenhouse gases is necessary for keeping our planet warm and habitable, excess greenhouse can have severe repercussions on life. Elevated earth temperatures can melt arctic ice which can lead to higher sea levels. This eventually could lead to flooding, food insecurity, extinction of many forms of life, and devastating weather conditions (Clark et al. 2016) (Battisti 2009). The increasingly adverse global climate changes dictate pressing needs to reduce the emissions of carbon dioxide. As a result, the chemical industry needs to abide by law enforcements of CO2 reduction including: Cap-and-trade and carbon tax policies (Stavins 2001).

One plausible way to reduce carbon dioxide emissions is to sequester the greenhouse gas into value-added products via different processing routes. Extensive research is continuously reported on novel synthetic routes to convert carbon dioxide into useful products. However, not all processing routes reported are profitable or even result in net emission reduction. For example, a processing route to convert carbon dioxide into methanol involves hydrogen as a reactant. Hydrogen is an expensive raw material which is usually obtained by steam reforming of fossil fuels or natural gas. To increase hydrogen yield, the steam reforming process involves the reaction of carbon monoxide and water vapor in a reaction known as the **water-gas shift reaction(WGSR).** The WGSR produces one mole of carbon dioxide for every three moles of hydrogen produced. Some questions here to consider: Are we really having net CO2 reduction? If yes, is the process profitable? If no, can the process be improved? What are the limits for CO2 fixture in this process?

**Course content: Process integration as a tool for sustainable design**

A chemical process design has to meet numerous criteria and address multiple challenges to be worth investing in. Some challenges include economic profitability, energy conservation, pollution reduction, and productivity increase. Optimizing these criteria in designing a new chemical process without compromising the process safety or the opportunities for future generations is commonly known as **sustainable design**. Sustainability balances the three basic objectives of any chemical process: profit, environment, and society. A sustainable process is a compromise for the three competing criteria.

Process integration is the systematic and methodical way for achieving sustainable design. The approach is holistic and consists of clearly defined activities for process design and retrofit. Process integration involves the following activities (Halwagi, 2012).

1. **Defining a clear target**: This step consists of explicitly defining a practical process target. Possible targets could be the reduction of certain discharge, increasing profit by X %, or increasing productivity by Y%.
2. **Targeting**: This step includes determining the limits and the opportunities of the process. In particular, targeting involves benchmarking the true potential of a certain criterion in the process. Although we may not have clear pathways about how we will be able to reach that limit, it is still useful to know the true capability of a process criterion. An example of targeting may include determining the maximum amount of CO2 fixed in a process, or the maximum yield of a certain product.
3. **Synthesis of alternatives**: At this step, the process input and outputs are clearly defined. The overwhelming number of solutions is determined and the flow sheet for the processing sequence is developed. Process synthesis is carried out at this stage to meet the set objectives.
4. **Selection of alternatives**: The process synthesis activities are completed in this step by selecting the optimum routes from the superstructure developed in the synthesis stage. Optimization software and tools are used to rank the competing solutions according to the set criteria. The step is followed by selection of the optimum alternatives.
5. **Analysis of optimum solutions**: Process analysis is carried out at this step. Simulation tools, empirical relationships and models are developed to test the actual performance of the selected solutions. In this step, the process inputs and process structure is defined while the process output is determined.

As illustrated, process integration is a multidisciplinary approach to achieve a clearly defined targets for sustainable design. This technique will be applied in the case study for carbon dioxide mitigation technique to solve for minimization of CO2 discharge into the atmosphere.

**Process Economics and Profitability**

Profit is the main driving force behind any chemical industry operation. There are numerous methods to determine early on in the process synthesis and design stages the potential economic viability of a process. An important stoichio-nomic indicator that can be used to determine the profitability potential is known as **Metric for Inspecting Sales and Reactants (MISR)** that can be expressed as follows:

MISR =

High values of the MISR ratio indicate that the products sell at a higher price than the cost paid to buy the reactants. This indicates potential profitability of the process, and thus higher values of MISR ratios are desirable. Processes with MISR values higher than unity value can be considered for more detailed analysis; while processes with less than unity are not economically viable. However, it is worth noting that a process with an MISR ratio higher than one cannot be considered automatically profitable. This is because when assessing the profitability of a process, several other factors come into account. Some other profitability factors include: utility costs, fixed capital investment, and variable operating costs. Nonetheless, MISR is a useful and quick method that can pinpoint whether it would be worth it to investigate further into a particular process.

A typical profit optimization function can be expressed as follows:

Profit (per annum) = Revenue from selling products – Cost of raw materials – Fixed capital investment per annum – operating costs per year

The fixed capital investment for a chemical plant is the cost of the fixed assets to start a new chemical plant. This cost incurs the charges for purchasing process equipment, land, piping, and instrumentation. The fixed capital cost is not paid in lump sum, but rather over installments over a set investment period. It is a typical practice for investors to borrow loans from credit bodies with certain interest rates, and then the fixed capital cost is divided equally upon the investment period.

The operating cost is a variable cost dependent upon the production. Such costs typically include utilities and labor. This cost is usually expressed in monetary value per a quantity of product.

**Case study**

The need to reduce and treat carbon dioxide emissions has become irreplaceable for the society. Carbon dioxide is a stable molecule that requires high activation energy to undergo chemical reactions. As a result, extensive research is taking place to investigate catalysts and reactions necessary for carbon dioxide activation. Numerous results are reported that show the chemical viability to transform carbon dioxide into useful chemicals via organic, inorganic, photochemical, and biological synthetic routes. This case study focuses on identifying and investigating the possible inorganic and organic synthetic routes of carbon dioxide that form useful products. The main aim of the case study is to use optimization tools to identify the synthetic routes that result in maximum profit and CO2 sequestration.

**Connections to Existing Core Curriculum**

In a report titled *The Engineer of 2020: Visions of Engineering in the New Century,* the National Academy of Engineers conveyed the need for sustainability education in engineering curricula as follows:

“It is our aspiration that engineers will continue to be leaders in the movement toward the use of wise, informed, and economical sustainable development. This should begin in our educational institutions and be founded in the basic tenets of the engineering profession and its actions.” (NAE, 2004)

This sustainability course encompasses many chemical engineering principles including mass and energy balance, thermodynamic equilibria, and plant economics. Although some of this knowledge base is usually taught in senior-level courses, the operating principles of this module are simple and can be learned while the student is taking the module. Nevertheless, this module can be best suited for senior-level chemical engineering undergraduate students.

**References**

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Stavins, Robert N. (November 2001). "Experience with Market-Based Environmental Policy Instruments" (PDF). Discussion Paper 01-58 (Washington, D.C.: Resources for the Future). Retrieved 2010-05-20. Market-based instruments are regulations that encourage behavior through market signals rather than through explicit directives regarding pollution control levels or methods.

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