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# Integration of Process Design and Intensification Learning via Combined Junior Course Project

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## ABSTRACT

We present the implementation of combined junior course projects encompassing three core courses: reaction engineering, separations, and process simulation and design. The combined project aims to enhance the vertical integration of process design learning through all levels of the curriculum. We design the projects to utilize novel modular process technologies (e.g., membrane separation) and to emphasize new process design goals (e.g., sustainability, decarbonization). Two example projects, respectively on green methanol synthesis and ethylene oxide production, are showcased for project implementation. Feedback from junior and senior students is also presented to motivate the development of such joint project in CHE curriculum. We will also discuss the challenges we hope to address to maximize student learning from this unique project.

**Keywords**: Education, Modelling and Simulations, Process Design, Process Intensification, Carbon Capture.

## INTRODUCTION

Chemical Engineering curriculum is well-recognized for its broad scope covering many core concepts with a wide range of engineering applications. Students typically acquire the fundamentals distributed over courses in the first three years while applying the entire body of knowledge to a capstone design project during the senior year. Given this, vertical integration of process design experiences through the curriculum[1-2] offers promise to help students develop a connected ChE knowledge map and foster critical thinking before starting senior design.

In this paper, we present our efforts on advancing junior-level design education, in particular, leveraging combined projects joint across three courses that students are taking in the Spring semester, namely Reaction Engineering, Separations, and Process Simulation and Design. The major goals of the combined project include:

1. Students work in teams to solve open ended chemical engineering problems.
2. Integrate topics and knowledge from multiple courses towards plant design and optimization.
3. Learn emerging new modular units (e.g., membrane) and integrate to existing process options.
4. Learn new process design goals including decarbonization, sustainability, etc.

## EXAMPLES OF COMBINED PROJECT

### Project 1: Methanol Synthesis using Captured $CO_2$ and Green Hydrogen

The Spring 2022 combined project is shown in Fig. 1, which involved the modeling, simulation, and optimization of an industrial-scale methanol synthesis process using captured $CO_2$ and green hydrogen. The $CO_2$ capture unit, which was the focus of Separations course, involved designing and optimizing a membrane-based process for $CO_2$ capture from natural gas combined cycle plant[3]. This enabled the students to be familiar with a relatively new separation technology as opposed to traditional sorbent-based processes. For the $CO_2$ hydrogenation reactor, the focus of Reaction Engineering course, students analyzed various reactor designs and operating conditions with an emphasis on the impact of recycle stream. This enabled the students to model a more complex reactor while investigating how the reactor design was influenced by the up/down process streams. Students also simulated and analyzed the entire flowsheet[4] as part of Process Simulation and Design course. Process design optimization strategies were proposed and investigated by students, assessed against multiple economics and sustainability metrics.

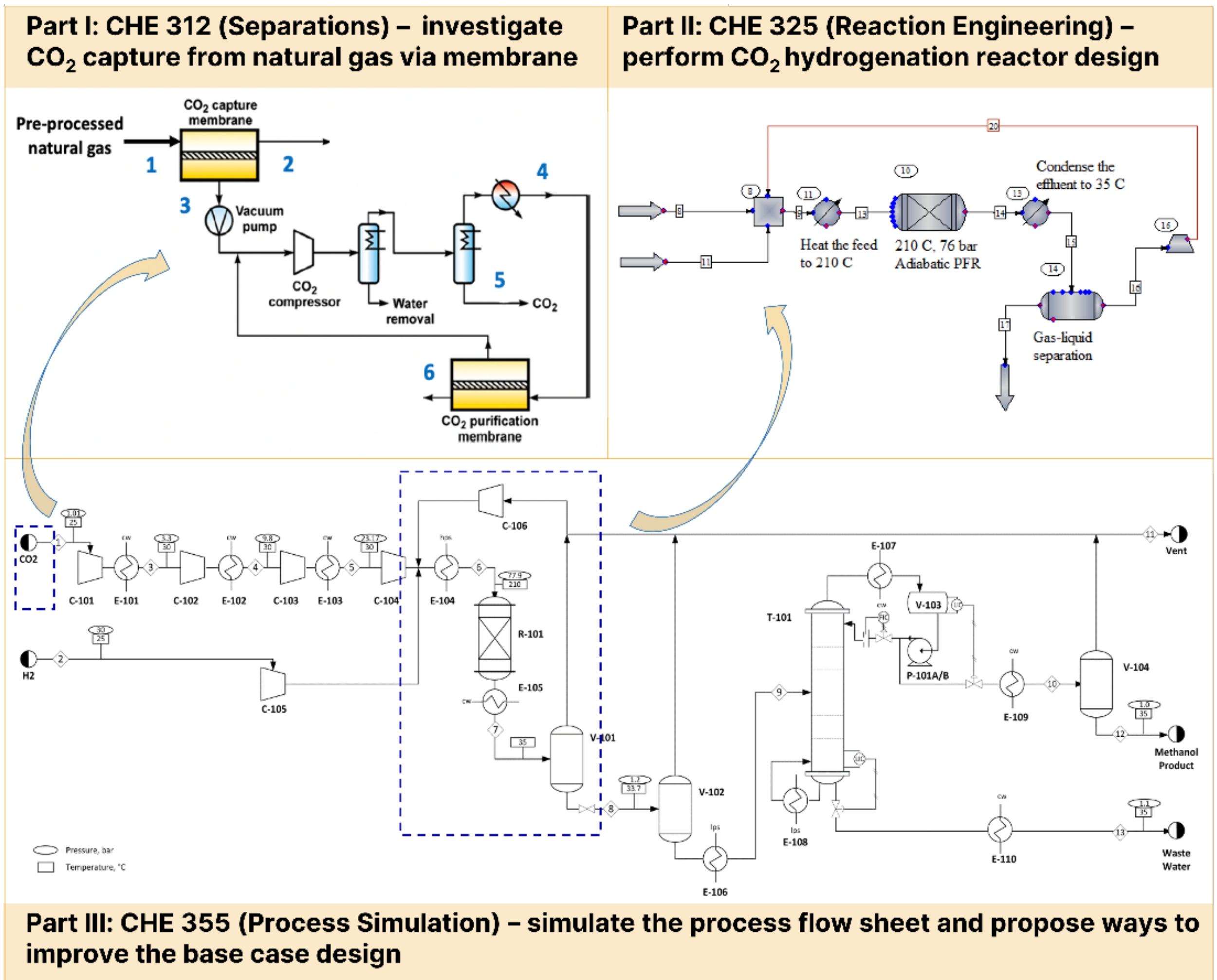


**Figure 1:** Combined design project for methanol synthesis using captured $CO_2$ and green hydrogen.

## Project 2: Ethylene Oxide Production

Fig. 2 illustrates the Spring 2023 combined project to design an ethylene oxide production plant via the direct oxidation of ethylene. The base case process design starts with compressing a mass amount of dry air which includes both nitrogen and oxygen. The multi-stage compressors are the major energy consumer in this process. The Separations course focuses on analyzing an alternative route in which oxygen is first separated from air via membranes before being sent to compressors. This enabled the students to quantitatively compare two process options, including a well-established process with high energy intensity and an emerging modular process where the large-scale commercialization is at an early stage. For the ethylene oxidation reactor, the focus of Reaction Engineering course, students compared the simulation using equilibrium-based reactor and kinetic reactor to understand the characteristics of this reaction. Students also searched for alternative catalysts from open literature, such as the use of promoters on the Ag catalyst to improve selectivity to the ethylene oxide product. This enabled the students to learn the impact of reaction kinetics on the design and optimization of this reactor unit as well as the integrated process systems. Students simulated and optimized the entire flowsheet as the focus of Process Simulation and Design course. They also analyzed the bottleneck of base case process design based on cost breakdown and investigated systems-level integration of the upstream membrane units.

## IMPLEMENTATIONS AND OUTCOMES

This section presents several examples to showcase student implementations for the green methanol synthesis project (Fig. 1).

### Separations

The Separations design project was focused on simulating a hollow fiber membrane-based carbon capture

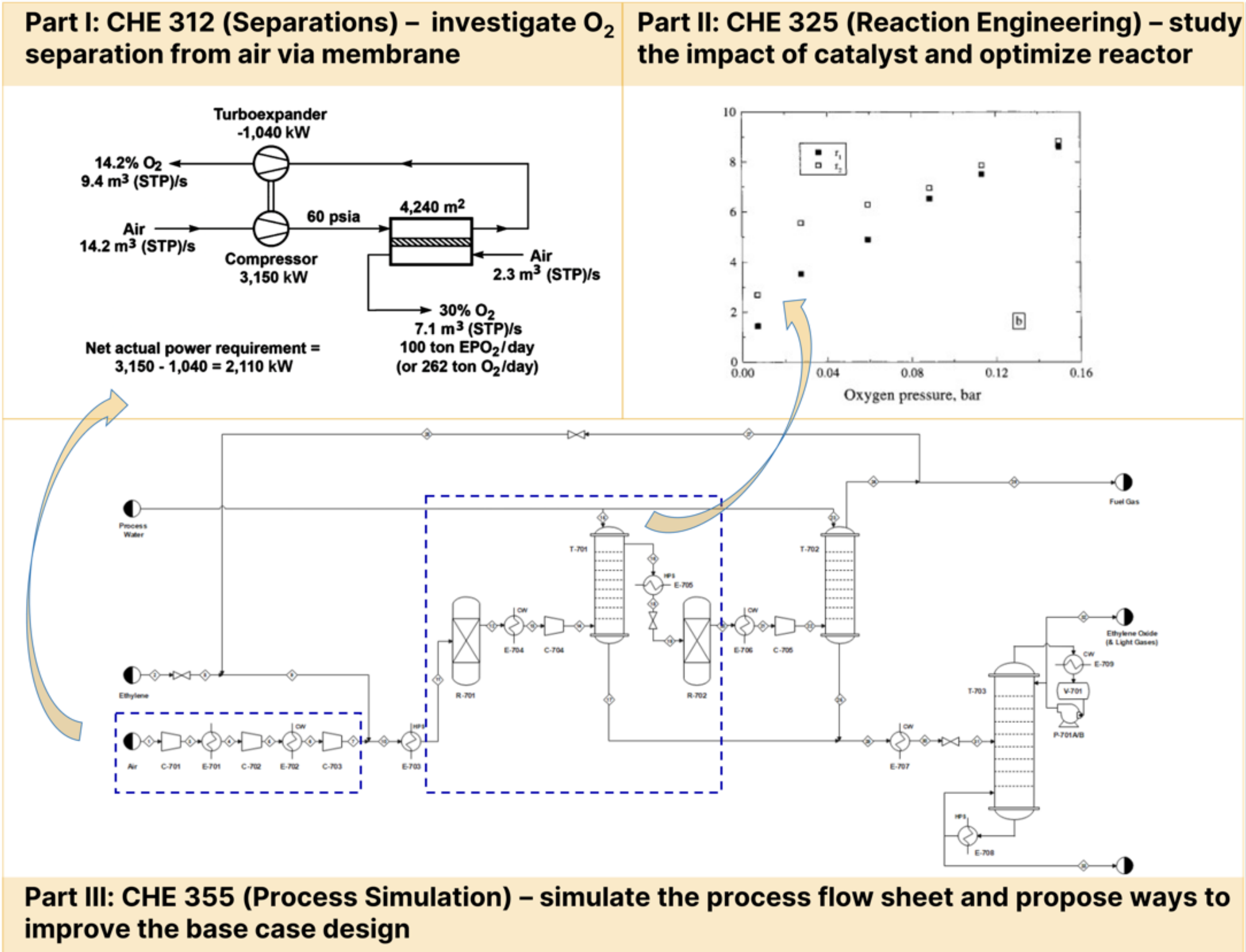


**Figure 2:** Combined design project for ethylene oxide production.

process, in conjunction with natural gas combined cycle (NGCC), i.e., primarily aimed at $CO_2/N_2$ separation. The project involved analysis of the effects of intrinsic membrane parameters ($CO_2$ permeability and $CO_2/N_2$ selectivity) on the overall system performance such as product quality, recovery, and membrane area. The membrane properties were chosen from prior experimental studies. Some preliminary calculations were expected to be done by students using the membrane separation principles covered during regular lectures. The students were also required to identify the input parameters (e.g., membrane performance, upstream/downstream pressure) which significantly affect the final product purity. Finally, the student groups were asked to identify improvement and possible modifications to the proposed system. Results from one representative group are shown in Fig. 3.

## Reaction Engineering

The Reaction Engineering design project section was focused on simulating the $CO_2$ hydrogenation reactor and investigating the impact of the recycle stream on reactor performance. The rate expressions for both methanol synthesis and the reverse water gas shift reactions were provided along with the corresponding kinetic parameters. These kinetic expressions were implemented into CHEMCAD by the students and compared the reaction section - including reactor, heat exchanger, flash vessel, and recycle – modeled with these kinetics vs a reactor at equilibrium. Students were asked to report selectivity and yield, as well as fractional conversion as a function of the reactor volume to optimize the reactor sizing. Additionally, they were asked to propose a reactor improvement based on either economic or performance metrics. As an example of the results, one project group results are shown in Fig. 4. This specific group used profit as the metric by which to conduct their optimization and determined the reactor volume based on maximum profit.

## Process Design and Simulation

The Process Simulation and Design project section was focused on simulating the entire flowsheet using CHEMCAD, which included (multi-stage) compression of the $CO_2$ and $H_2$ feed streams, $CO_2$ hydrogenation reactor, and a series of separation units (flash and distillation

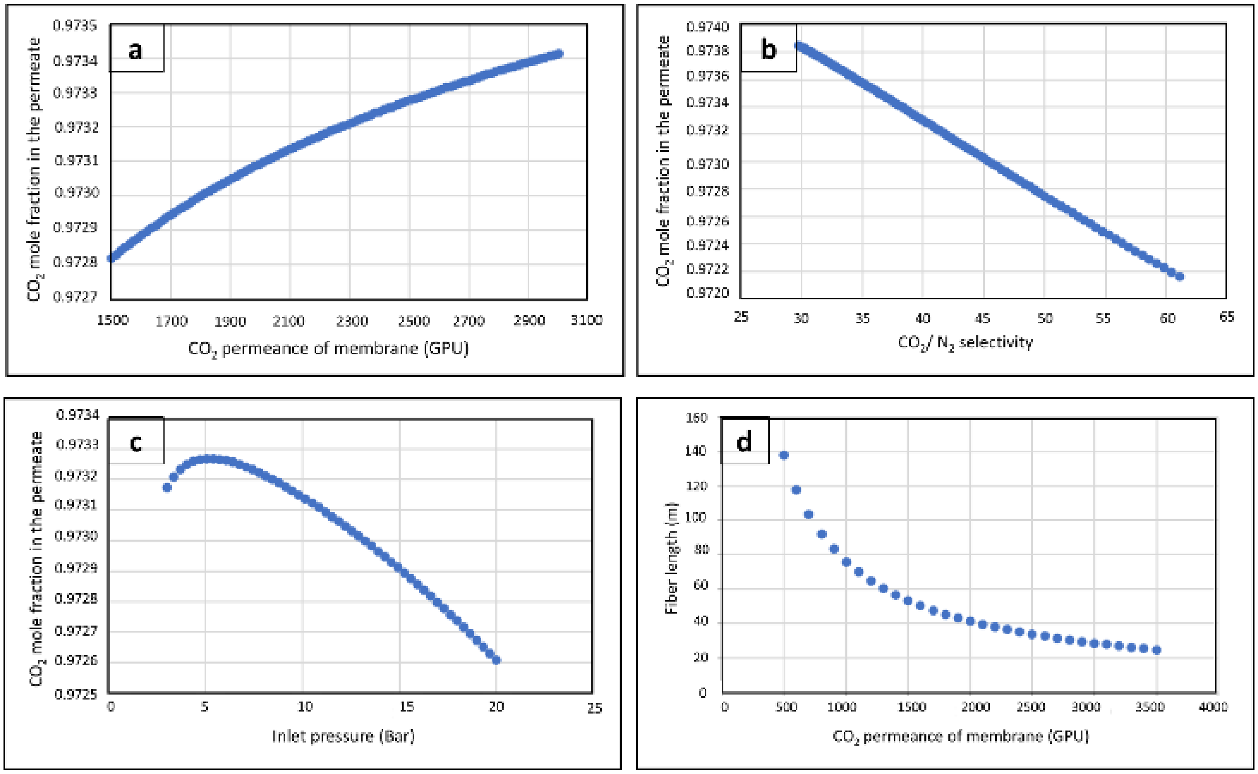


**Figure 3:** Effects of (a) $CO_2$ permeance, (b) $CO_2/N_2$ selectivity and (c) Inlet pressure on permeate quality and (d) effect of $CO_2$ permeance on the fiber length.

columns). Students were also required to perform equipment sizing and calculate the equivalent annual operating cost (EAOC) to identify the process design bottlenecks. On this basis, students would propose and implement two major areas for process improvements. Fig. 5 presents an example of the improvements by one of the design groups, where they applied heat integration utilizing the high temperature reactor effluent to heat the inlet streams respectively to reactor and distillation column. Additionally, they added a membrane module to recover hydrogen from the vent stream. As this project assumed the use of green hydrogen, the raw material cost took up more than 80% of base case EAOC. The recovery of remaining $H_2$ would effectively reduce the cost. The students proposal of using a membrane for downstream gas separation also well justified the efficacy of this combined project to bring emerging modular intensified process technologies to the toolbox of next-generation chemical engineers. To address the trade-off between sustainability and economic competitivity as illustrated by this green methanol process, one design group explored the impact of carbon tax.

## STUDENT FEEDBACK

After the second year of project implementation, surveys were conducted for both project cohorts of students. The survey administered to the junior students who had just completed the project (2023 project on ethylene oxide production) focused on how the project helped them develop skills and apply technical content from the courses. The survey administered to the senior students, who had completed the joint project approximately one year prior (2022 project on methanol synthesis), focused on how the project prepared them for senior design.

### Junior Survey on Combined Project

The primary survey question investigated whether students felt the joint project helped them to practice material from each of the three courses, shown in Fig. 6.

Most students felt that the joint project helped them practice material from the Process Design course, with a strong majority answering “very much”. For the Separations and Reaction Engineering courses, however, responses were more distributed with approximately equal numbers of students responding 3 (neutral), 4, or 5 (very much).

Additionally, students were asked to compare their skills before and after working on the junior design project across a range of areas, including technical skills such as process design and optimization as well as skills

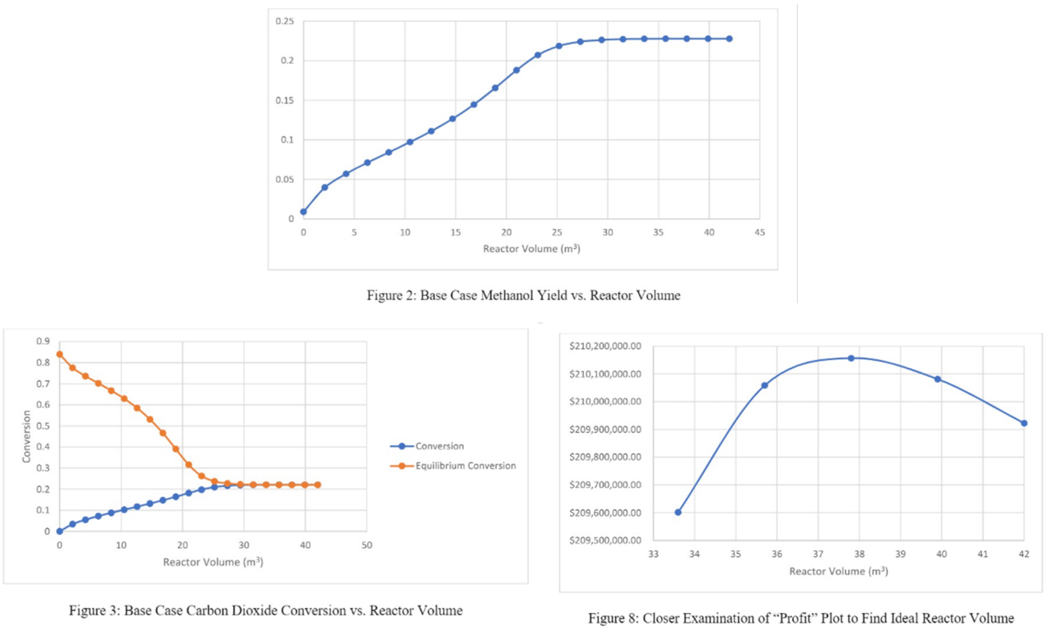


**Figure 4:** (Top) Methanol yield as a function of reactor volume, (bottom left) conversion and equilibrium conversion as a function of reactor volume, and (bottom right) process profit as a function of reactor volume to determine the optimum reactor size.

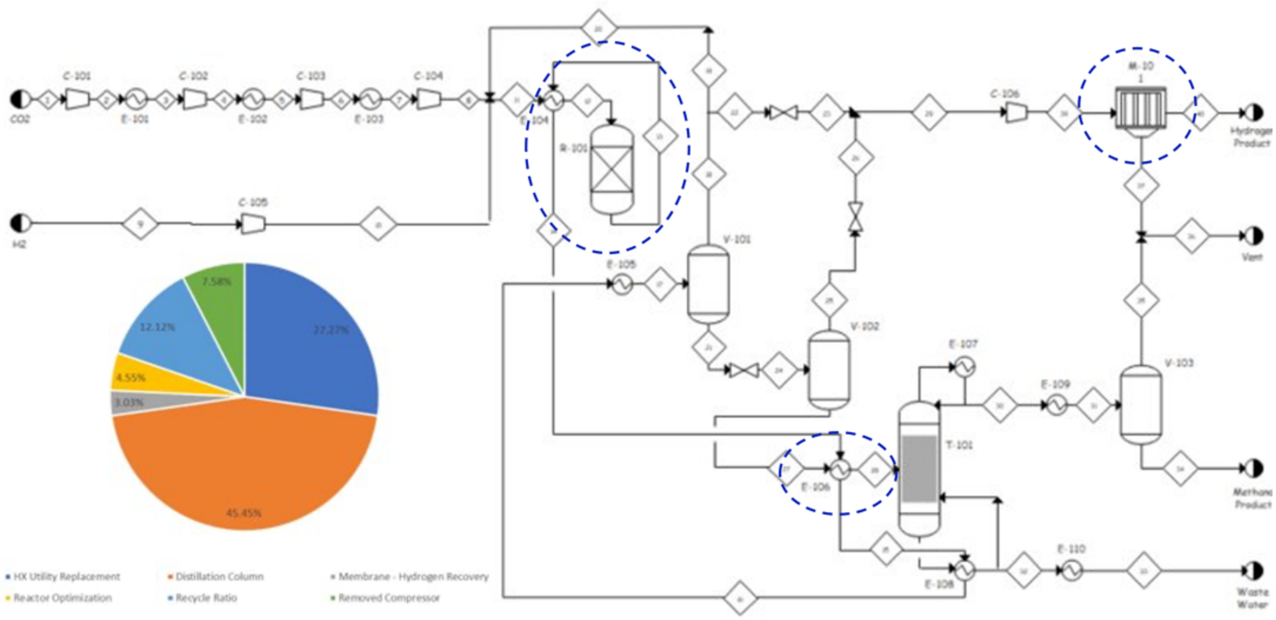


**Figure 5:** Process design improvements via heat integration and membrane-based hydrogen recovery.

such as teamwork, communication, and creativity. The results are shown in Fig. 7, with the left of each bar indicating before the project and the right of each bar indicating after the project.

While all skills showed an improvement after participating in the design project (indicated by more green and blue and less red/orange/yellow), the most significant improvements were observed for the technical skills. In reflecting on the beginning of the class, at least half the class rated themselves as having poor, fair, or good skills in process/single unit design and optimization. After participating in the project, the vast majority of the students reported their skills in these areas as very good or excellent. Improvements to group work, communication, and other similar skills were less drastic.

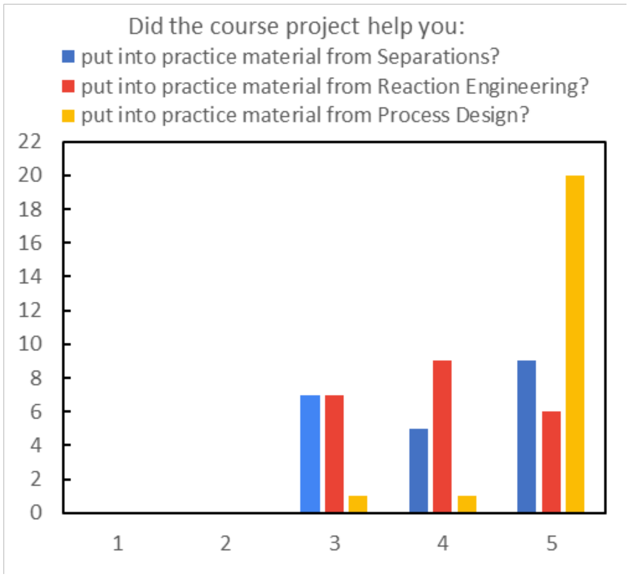


**Figure 6:** Responses from junior students to “Did the course project help you put into practice material from Separations (blue), Reaction Engineering (red), and Process Design (yellow)?” Responses were given on a scale of 1 (not at all) to 5 (very much).

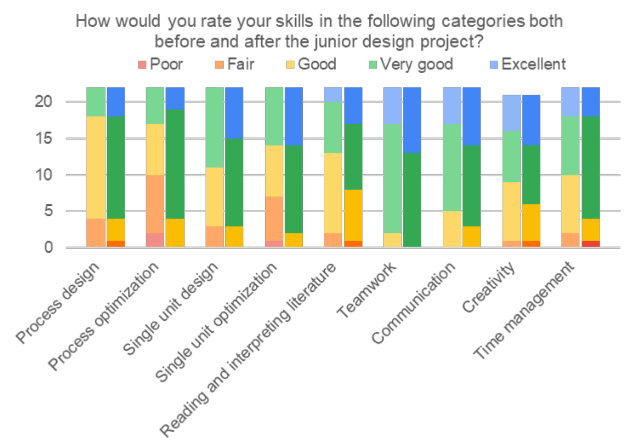


**Figure 7:** Responses from junior students on their skills in a variety of topic areas before (left, faded) and after (right, darker) working on the junior design project. Responses were given on a scale of poor, fair, good, very good, and excellent.

## Senior Survey on Preparation for Capstone Design

The senior students who participated in the first implementation of the joint project in Spring 2022 were surveyed about their experience in Spring 2023. This survey served to assess their perception of preparation for their senior design course, as well as their retrospective perception of how well the project helped them practice material from each of the junior level courses. Most students reported a neutral or positive experience of working on the project, however the perception of preparation for senior design was mixed. Students reported an average of 3.4 (out of 5) indicating they felt that the junior course project somewhat prepared them for senior design.

Additionally, when asked if the joint course project helped students practice material from each of the three courses, a range of responses were given. Notably, the students reported that the project helped them practice course material to a lesser extent than the junior responses, indicating that the project modifications between implementation in 2022 and 2023 better connected the course content and project. Similar to the responses from the junior class above, the students found that the project helped them put into practice material from Process Design to a greater extent than Separations or Reaction Engineering.

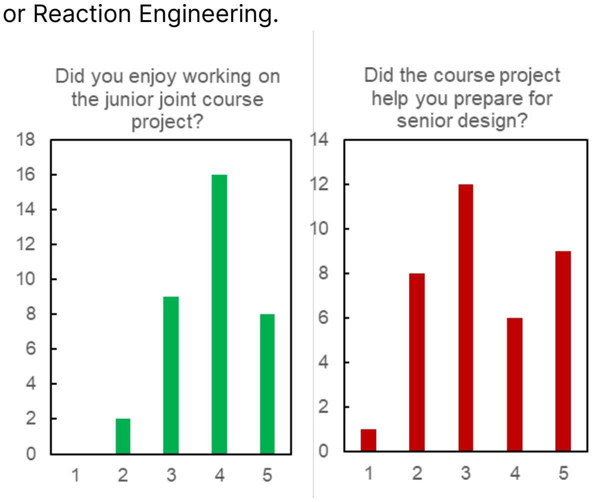


**Figure 8:** Survey results for seniors, responses collected approximately one year after completing the joint junior course project. Scale of 1 (not at all) to 5 (very much).

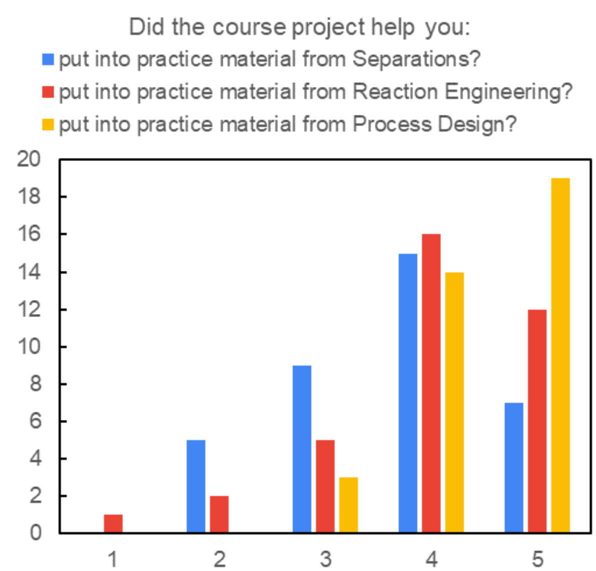


**Figure 9:** Survey results for seniors, responses collected approximately one year after completing the joint junior course project. Scale of 1 (not at all) to 5 (very much).

### Select Student Comments

#### Comments from seniors who took CHE 355 in Spring 2022 (surveyed a year later)

*Q → What was the most interesting/enjoyable part of the junior course project?*

**Response:** The integration of a single topic between all of our core classes (since it reflected more of a real-world process design project)

*Q → What was the most challenging part of the junior course project?*

**Response:** Finding a true optimum case because so many factors + process units depend on each other

#### Comments from juniors who took CHE 355 in Spring 2023 (surveyed at the end of semester)

*Q → What was the most interesting and/or enjoyable part of the project?*

**Response 1:** The most interesting part of the project was finally integrating all of the information we've learned into one project instead of a bunch of little bits and pieces.

**Response 2**: Seeing how much money that can be saved with implementation of simple optimizations was very interesting.

## CONCLUDING REMARKS

In this paper, we have introduced our development of combined junior process design project across reaction engineering, separations, and process simulation and design. Two project examples are presented which strive to integrate the knowledge from different courses and highlight the increasingly important process design goals such as sustainability and decarbonization. It is worth highlighting that the implementation of such combined course projects can be greatly benefited by, while not restricted to the availability of, a specialized process design course at junior level. Based on student feedback, we aim to address the following key points to continuously improve the combined project in future semesters:

- Emphasize systems-level optimization and its interactions (or trade-offs) with single unit optimization.
- Emphasize process design and optimization with simultaneous considerations of multiple objectives (e.g., economics, carbon footprints, water usage).
- Arrange training workshops on Aspen and custom modeling to prepare students for senior design with an enriched set of simulation tools and skills.
- Integrate graduate student teaching practice to train next-generation process design educators.


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