STRATEGIES FOR CHEMICAL PROCESS DESIGN: A SUSTAINABILITY-BASED APPROACH

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Abstract

"Team Strategies for Engineering Design" is a third-year undergraduate course in our chemical engineering curriculum where student teams develop leadership and management skills while applying decision-making methodologies to process engineering design. Typical deliverables for this course include process flow and piping & instrumentation diagrams centred on developing processes under safety and environmental considerations. This work describes the design and implementation of our revamped version of this course, which consists of four (4) engineering pillars: (i) process description and heat & material balance, (ii) process drawings, (iii) sizing and safety, and (iv) circular economy. Sustainability is discussed in all deliverables and tasks, with a special emphasis on minimizing waste and energy consumption, complying with environmental regulations, performing plant risk assessments, and discussing life cycle assessments. Data-based modelling for prediction and optimization is also taught as a complementary tool for traditional process simulation approaches. Moreover, the corresponding chemical processes are linked to a vertically integrated framework of our curriculum, which combines core engineering concepts and process design around biodiesel plants in different courses of our program. Finally, the teams submit a "strategies report" (engineering logbook), where all engineering strategies to achieve the process engineering goals are summarized and discussed. With this revamped version, we expect to guide students to assume responsibility for designing sustainable chemical processes while enhancing students' career readiness.

Keywords: Curriculum integration, chemical process design, sustainability.

Introduction

The integration of sustainability-related topics in the chemical engineering curriculum has been strategized in different teaching approaches and in different courses, including fundamentals [1], introduction to industrial case studies [1], life cycle assessment (LCA) [2], and use of green engineering tools and computer-aided tools in chemical process design [3]. When clustering these integration strategies, they fall into the Body of Knowledge for green engineering in chemical product and process design, which includes three elements [4]: (i) framing the challenge (e.g., emissions, risk, and life cycle analyses, and environmental legislation), (ii) assessment and design (e.g., applying general principles at unit operation scales), and (iii) system perspectives (e.g., integration of materials and energy flows among various unit operations) [4]. While traditional engineering education is based on problem-solving, data analysis, and modelling [5], sustainability engineering education must incorporate additional key elements such as decision-making and teamwork [6], [7]. Engineering capstone courses integrate skills and competencies in both domains, traditional and sustainability-based engineering education, as they require students to apply fundamental knowledge in transport phenomena, kinetics, heat transfer, and soft and social skills [7]. A sustainability-competence approach was implemented in a capstone course by [7] including proposing alternatives for energy integration in process design, identification, and quantification of the industrial needs, identifying opportunities for design optimization and automation, as well as the use of numerical methods for process design optimization, among others [7].

A sustainability integration strategy can be assessed at least in two dimensions when analyzing process design [8]: (i) economic, with cost-effective solutions and added value of chemical routes; and (ii) environmental, by minimizing energy consumption, emissions, effluents, and waste. Moreover, safety indices also contribute to assess sustainability when deciding over chemical process routes, for which different approaches have been implemented, including Hazard and Operability Study (HAZOP), WHAT-IF, and RAM study (reliability, availability, maintainability) [9], [10]. Additional, indicators of "circularity" (within a circular economy framework) can strengthen this integration, as we look at chemical process design for zero waste, by reusing, recycling and/or renewing materials [11].

At the University of Toronto, sustainability topics have been vertically integrated into our chemical engineering undergraduate curriculum through analyzing and/or designing a biodiesel plant, whose elements/unit operations/principles have been discussed in several courses over different years. In addition to this integration strategy, we have three design-related courses where sustainability has been addressed: (i) *CHE324 Process Design* is a third-year course that introduces the philosophy of chemical engineering design projects, including material and energy balances, design of unit operations, equipment specifications, and development of piping and instrumentation diagrams. Sustainability topics are covered by introducing safety, health, and environmental regulations and focusing on the process design to develop safe operating procedures; (ii) *CHE334 Team Strategies for Process Design* follows CHE324; it is a third-year course emphasizing team development and problem-solving related to process safety in engineering design. Typical deliverables for this course include process flow diagrams and piping and instrumentation diagrams centred on developing processes under safety and environmental considerations. Finally, in (iii) *CHE430 Plant Design*, students work in teams to design plants (for specific real-world clients) and analyze their feasibility. Students' understanding of sustainability-related topics in these courses has been assessed by the teaching team through tasks including HAZOP and inherently safe designs (e.g., adding pressure relief valves in different equipment/unit operations), while minimizing Capital Expenditure (CapEx) and Operational Expenditure (OpEx).

CHE334 is a course bridging CHE324 and CHE430, where team strategies, including working in teams, leading and managing teams, and providing students with decision-making methodologies for successful teams, are taught in engineering design. It is focused on team development and problem-solving and is associated with the main process engineering practices, including process safety and engineering design. Pre-requisites include CHE249 Engineering Economic Analysis, CHE324 Process Design, and CHE332 Reaction Kinetics. Students typically enrolled in it while taking CHE311 Separation Processes, and CHE333 Chemical Reaction Engineering, a synergy required to complete the engineering design components of CHE334. While not being formally pre-requisites, other core courses such as CHE210 Heat and Mass Transfer, CHE211 Fluid Mechanics, CHE323 Engineering Thermodynamics, CHE322 Process Control, as well as CHE220 Inorganic Chemistry, CHE213 Organic Chemistry and lab components through CHE204/205/CHE304/305 Chemical Engineering and Applied Chemistry laboratory I to IV, are relevant to the problem-solving tasks developed by the students.

In this work, we describe the design and implementation of our revamped version of the course CHE334, a course bridging between CHE324 and CHE430, and consists of four engineering pillars: (i) *process description and heat & material balance*, (ii) *process drawings*, (iii) *sizing and safety*, (iv) and *circular economy*. Our sustainability integration approach is based on coupling (i) sustainability-related topics in all process design deliverables, (ii) using data-based modelling for prediction and optimization as a complementary tool for traditional process simulation approaches, and (iii) providing students with chemical processes linked to a vertically integrated framework of our curriculum, around biodiesel production concepts taught in different courses of our program.

Methodology

This section describes the sustainability-based approach and the consequent revamp of the course *CHE334 Team Strategies for Process Design*.

The CHE334 lecture (L) schedule and deliverables are included in Tables 1 and 2.

Table 1. Previous CHE334 lecture schedule

Lecture	Description
L1	Introduction to the course and teaching team
L2	Teamwork expectations and evaluations
L3	Process flowsheet discussion
L4	Equipment selection and sizing
L5	Process simulation
L6	Safety in design
L7/8	Process economics
L9	Technical writing workshop
L10	Course wrap-up

Table 2. Previous CHE334 deliverables (A)

Assignment	Description	Breakdown, %
A1	Team charter and project charter	4
A2	Individual and team performance assessment (ITP 1)	2
A3	Safety discussions	2
A4	Technology summary	1 (bonus)
A5	ITP 2	2
A6	Final report submission	70
-	Teamwork assessment	20

Previously, the main course assignment was completed in groups of five students each. Every project statement provided student with stoichiometric equation(s), kinetics rate expression, plant capacity, and key reference(s). The CHE334 projects fell into four categories: (i) commodities, involving the design of continuous gas-liquid reactors; (ii) specialties, typically batch processing to produce lower volume but higher value-added specialty chemicals; (iii) environmental, and (iv) natural resources-hydrometallurgy, including processes to extract metals from their ores using aqueous systems.

Part of the course deliverables were accomplished in the tutorial sessions, where students met with their Teaching Assistants (TA) to complete actions (defined by the team) to meet specifications and prepare the deliverables.

For the revamped version of CHE334, we strategized a sustainability integration approach based on coupling (i) sustainability-related topics in all process design deliverables, (ii) using data-based modelling for prediction and optimization in addition to process simulation, and (iii) alignment with the vertically integrated framework of our curriculum. The corresponding workflow and rationale for our strategy are as follows:

Process selection. This selection shall be aligned with our vertical integration of biodiesel processes in different courses in our curriculum, from fundamentals (e.g., Heat and Mass Transfer, where heat exchangers from these plants are sized) to laboratories (e.g., Unit Operations, where several experiments around the synthesis, transport, and distillation of biodiesel are conducted). Students, therefore, are already familiar with these production processes.

Process engineering pillars. These pillars shall cluster process engineering deliverables in the industry, namely, process description, process flow diagrams, piping and instrumentation diagrams, equipment sizing, safety studies, and economic analysis, in alignment with the learning objectives of the course.

Sustainability topics. Once we have identified the process engineering pillars, we shall prioritize relevant sustainability topics to be included in each cluster and define the corresponding scope per deliverable.

Process deliverables. They shall be defined in alignment with the process engineering pillars and learning objectives of the course.

Synergy with the courses CHE311 Separation Processes and CHE333 Chemical Reaction Engineering is required to complete the engineering design components related to distillation column and reactor sizing. For instance, the reactor sizing component of D2 is being evaluated by the CHE333 teaching team.

Once we had the new course's structure and content, we modified lectures and tutorials accordingly. Lectures (one hour per week) gave students the fundamentals to prepare all the deliverables. In parallel, tutorials (two hours each per week) provided students with guided tasks to apply theory in a generic scenario and on their specific process design.

Results

We selected two biodiesel production processes for our revamped course: an alkali-catalyzed process to produce biodiesel from virgin oils (Project "A") [12], and a homogeneous acid-catalyzed process to produce biodiesel from waste oils ("Project B") [13]. The fundamentals for their process simulations, and the preliminary heat and material balance, kinetics, equipment sizing considerations, and process flow diagrams are provided in the corresponding references [12], [13]. Half of the groups were assigned to work on Project "A' and the other half on Project "B".

We identified four engineering pillars, named *process description and heat & material balance, process drawings, sizing and safety,* and *circular economy*. The pillar *process description and heat & material balance* set the basis for understanding the chemical process and quantifying the influx and outflux of material and energy (process and utility streams, waste/emissions, and energy consumption). The pillar *process drawings* included the most important process engineering diagrams to be delivered in any engineering project: the process flow diagram (PFD) and piping and instrumentation diagram (P&ID). The pillar *sizing and safety* focused on sizing process equipment such as distillation columns, reactors, and miscellaneous equipment (heat exchangers, pumps, line sizing, and pressure safety valves). The pillar *circular economy* was defined around two key factors ensuring circularity: economic analysis and lifecycle assessment.

CHE334 now includes four deliverables encompassing the previous engineering pillars: (i) D1: process drawings (process flow diagram and piping and instrumentation diagram), (ii) D2: sizing and safety (equipment sizing – distillation, reactor, heat exchanger, pump, pipes, pressure safety valve; data-based modelling for prediction and optimization; hazard identification), (iii) D3: circular economy (CapEX/OpEX, and lifecycle assessment), and (iv) D4: strategies report.

In D1, the students were asked to develop the PFD of the entire plant, and the P&ID of a main equipment (either reactor or distillation column). The PFD and P&IDs had to consider the inclusion of pressure safety valves (PSVs) and other safety considerations (e.g., bypasses, check valves, etc.). The development of these diagrams was based on previously preparing the process description and process simulation (prepared, checked, but not submitted for grading) to get relevant information about the heat and mass balance, process flow, as well as to preliminary strategize on minimizing heat consumption, waste, emissions, and other environmental design constraints.

In D2, the students were asked to perform equipment sizing of reactors, distillation columns, heat exchangers, pumps, PSVs, etc. This sizing was typically supported using process simulation, heuristics, and engineering standards. A data-based modelling approach was introduced, where students generated data from the simulation software (via a sensitivity analysis), fit data analytics/machine learning models (e.g., response surface method), and predicted key variables around one unit operation, looking at minimizing heat consumption, waste, and emissions, while maximizing yield and/or purity of products. Finally, a hazard identification (HAZID) study completed this deliverable, where potential threads and hazards were identified for their respective processes.

In D3, the students were asked to prepare an economic analysis (CapEX and OpEX), and a literature review regarding lifecycle assessments for biodiesel production processes, focusing on contrasting circularity indicators (e.g., consumption indicators, waste and emissions flow rates).

In D4, the students were asked to summarize all the strategies in an engineering logbook regarding the development of the deliverables D1 to D3, including assumptions, research approaches to fill information gaps, deviations/errors, sensitivity analysis, and circularity indicators.

To support the successful development of all deliverables, we modified the content and schedule of lectures and tutorials accordingly. Figure 1 shows the mapping between deliverables, lectures/tutorials, and deliverables breakdown of our revamped version of CHE334.

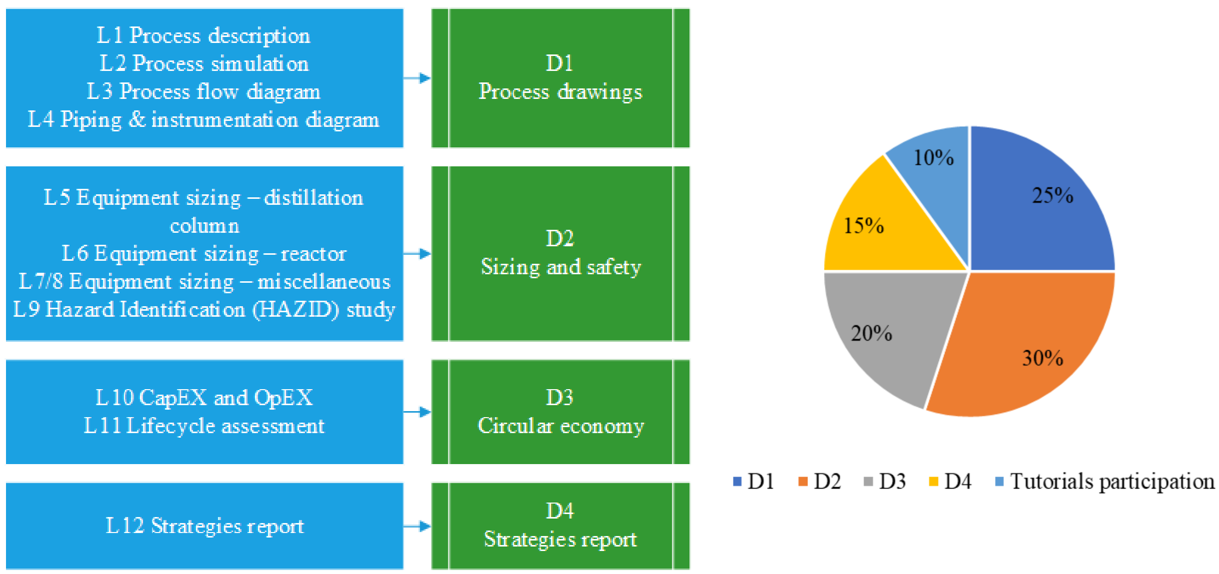

Figure 1. Mapping between deliverables, lectures/tutorials, and deliverables breakdown

Lectures L0 to L2 were sequentially designed to facilitate preparation and understanding of the project and all deliverables, while L3 and L4 were designed to support the development of D1; L5 to L9 for D2, L10 and L11 for D3, and L12 for D4.

Consequently, tutorials T1 to T12, mapped with L1 to L12, were designed to support the development of the deliverables. In the first hour of each tutorial session, the teaching assistant (TA) reviews generic applications of theory from the lectures (e.g., shortcut/rigorous distillation for simulation and sizing purposes). In the second hour, the TA provides students with guidance to work on their project (“A” or “B”, as assigned), for the required upcoming deliverable.

A comparison between the previous and revamped versions of CHE334 is shown in Table 3.

Table 3. Comparison between the previous and revamped versions of CHE334

Item	Previous version	Revamped version
Number of lessons	10	13
Nature of lessons	Not necessarily chronological	Chronological in preparation for partial deliverables
Number of projects	22 (Winter 2023), 1 per team	2 (Winter 2024), 11 teams per project
Sustainable-related projects, %	25	100
Integrated projects with curriculum (biodiesel), %	0	100
Tutorials’ support strategy	Support for the project	Lecture application and support for the project
Number of deliverables	6	4
Nature of deliverables	Mostly concentrated in the final report; strategies-related tasks during the semester	Process engineering-related deliverables split into three partial deliverables; summary of team strategies in D4
Sustainability-related content per deliverable, %	Mostly safety-related, 10% (P&ID, for instance)	Included in all lectures, tutorials, and deliverables (~ 35% of marks, as per rubric)

The main changes between the previous and revamped versions of CHE334 are the noticeable increase in sustainability-related projects, while reducing the number of distinct projects, and the full integration of the current projects with the vertical integration of biodiesel plants in our curriculum. The number of deliverables was reduced from six to four; all the deliverables were process engineering-related and split into three instead of a concentrated deliverable (final report submitted at the end of the semester). Moreover, as per our rubric, sustainability-related content was added to all deliverables and subtasks, accounting for approximately 35% of the marks.

In terms of circularity, a key pillar in our revamped version of CHE334, is quantitatively assessed by economic indicators (CapEx and OpEx), typical metrics such as percentage of recyclability and utilities/energy consumption, and qualitatively by discussing LCAs of different biodiesel production (assumptions, calculation procedures, and carbon footprint).

We believe that this revamped version of the course will guide students to employ principals and a framework for design of sustainable chemical processes. Furthermore, as the future chemical engineering workforce must design and enforce sustainable chemical processes, we believe this approach enhances students' career readiness. The effectiveness of this revamped version will be assessed with a testing plan that includes (i) different surveys conducted at the end of CHE430 (in the following semester), where students will qualitatively assess their perceptions about the effectiveness of CHE334 in bridging CHE324 and CHE430; (ii) and longitudinally gathering data from deliverables (both in CHE334 and CHE430) from which we may identify (and also compare with previous years) process optimization and circularity strategies/indicators when designing chemical plants, such as waste/emissions disposal, stream recycling, and co-generation.

Future work will include further efforts to implement machine learning tools and sustainability-related topics when designing chemical processes, looking at a broader approach to process optimization and circularity.

Conclusions

In this work, we describe the design and implementation of our revamped version of the undergraduate course CHE334 *Team Strategies for Process Design*, now entirely focused on sustainability for process design, and supported by four (4) engineering pillars: (i) *process description and heat & material balance*, (ii) *process drawings*, (iii) *sizing and safety*, and (iv) *circular economy*. The deliverables were designed to map with these pillars, while sustainability-related topics were included in all lectures, tutorials, and deliverables. Two biodiesel plants were selected for process design purposes, aligned with the vertically integrated framework of our Chemical Engineering curriculum. We believe that this revamped version will allow students to learn and apply sustainability-related principles when designing chemical processes, guiding them through a framework for implementation of such designs, while enhancing students' career readiness. Future work will introduce additional machine learning tools to enhance circularity in chemical process design.

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