Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale, Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

Integrated Project in the Master of Chemical Engineering and Materials Science at the University of Liège

Marie-Noëlle Dumont[a*], Marc Philippart de Foy[a], Grégoire Léonard[a]

[a] Department of Chemical Engineering, Faculty of Applied Sciences, Campus Liège Sart-Tilman, University of Liège, Belgium
* Corresponding Author: mn.dumont@uliege.be

ABSTRACT

The Integrated Project in the Master of Chemical Engineering and Materials Science at the University of Liège (ULiège) aims to consolidate technical knowledge and promote the acquisition of soft skills by integrating various chemical engineering disciplines. The project focus on the design of an industrial process and is divided into five parts: individual work on mass balances and literature reviews, detailed modeling of thermodynamics and key unit operations, sensitivity studies, process integration, and report to a general audience. Key learning outcomes include developing critical thinking, addressing complex multidisciplinary topics, and understanding the role of science and technology in society. Students enhance their soft skills in project management, teamwork, and effective communication in English. Regular interactions with industry and academic experts, along with support from the ULiège Soft Skills Team, ensure comprehensive development. Evaluation includes both technical and soft skills assessments, with individual and group performance contributing to final grades. This project, running for several years, is highly regarded by students for its rigorous and instructive nature, preparing them well for their future careers.

Keywords: Education, Process Design, Modelling and Simulations, Interdisciplinary

INTRODUCTION

In many universities, courses are given independently of each other and it can be observed that students tend to focus on each course and each exam separately, missing the overarching links between disciplines. However, integration into applied projects of different but related disciplines (such as catalysis, reaction engineering, chemical thermodynamics, separation processes or process system engineering among others…) is key for the training of future chemical and process engineers. Indeed, most chemical processes include reaction, separation and/or purification steps, pumps and/or compressors, heat exchangers… However, modeling these is only possible with the choice of an appropriate thermodynamic method and adequate kinetics. It is thus important that students are taught these disciplines and are able to integrate them for designing a relevant and efficient process, while justifying each choice and simplification. This approach is called for by industry, international education evaluators, and often by university authorities as well [1].

The project described in the present paper forces students to consider different disciplines as part of a coherent whole necessary to solve a given process design problem inspired by an industrial case study. Previous work has shown that process design is being taught in most Chemical Engineering curricula, and that it often includes teamwork activities in addition of individual mastery of the disciplines [2]. A recent work has surveyed the practices and the usual teaching methods regarding process design, evidencing the central importance of this topic in the chemical engineering education. It also highlighted common lines but also differences in approaches among universities [3]. In this paper, we present the Integrated Project offered to chemical engineering students at the University of Liège. We first describe the general context of the project and its objectives. Then, the teaching methods for technical skills are presented following the yearly progression of the work, and a specific focus set on soft skills development is highlighted.

PROJECT'S CONTEXT AND OBJECTIVES

This project is offered to senior students in

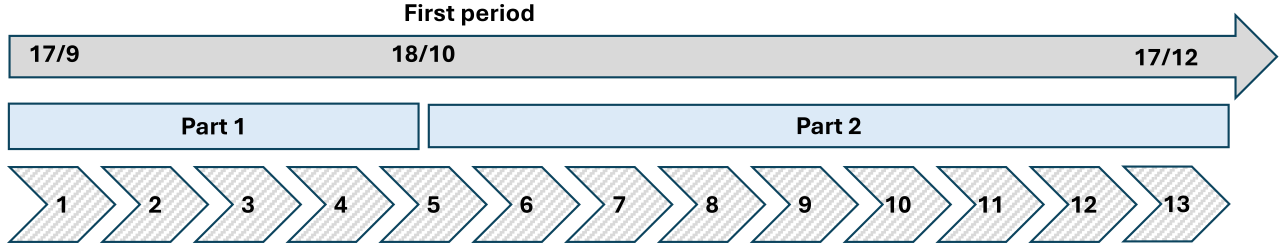

Figure 1: Timeline of the Integrated project at the University of Liège, Fall Semester

Chemical Engineering and Material Science at the University of Liège, i.e. a number of students usually ranging between 10 and 20. It was designed about 10 years ago and has evolved with the objective of confronting students with a less academic situation, more akin to what they will encounter in the industrial world. Groups are defined randomly, although the teaching team may intervene to make sure that the final student distribution respects some equity principles with respect to the student's background, e.g. Erasmus students are reasonably split among the groups. A new theme is proposed each year by a different industrial expert identified among the Department's network and who is accepting to provide some follow-up during the year. The initial definition is extremely broad: "propose a process to produce XX tons per year of YY product with ZZ purity." The technical key learning outcomes for the project are listed as follows [4]:

- Consolidate technical knowledge by integrating and linking the different disciplines of chemical engineering and integrate these disciplines within one unique project.
- Acquire critical thinking and ability to challenge and validate assumptions made. This includes the acquisition of a gut feeling for orders of magnitude typical of engineers.
- Address complex and multi-disciplinary topics centered on chemical industry.
- Develop knowledge about current hot topics in chemical engineering and increase the awareness about the role of science & technology in society.
- Use powers of judgment as engineers in order to work with complex and possibly incomplete information, to recognize discrepancies and to deal with them
- Recognize the need for information, find and provide information

Beyond the process design and the integration of technical skills, the development of soft skills is another major goal of this project. There, the key learning outcomes are also presented to the students, as follows [4]:

- Ability to work in large groups (between 7-12 students, random selection of members).
- Management of project and deadlines.
- Writing of technical reports in English, with written feed-back from teachers after each report.
- Communication to scientific and non-scientific audience: technical presentations to teachers, and final presentation to a larger audience with general engineering background.
- Communication in English, written and oral (all group members must talk).

The Integrated Project spans the entire academic year, from the first week of classes in September to the last week in May, with a break during the exam session from the end of December to early February. Each project is handled by a group of 6 to 12 students and accounts for 10 credits in an academic year that contains 60 credits. In this paper, we illustrate the Integrated Project of the 2024-2025 academic year, which is dedicated to the synthesis of Vinyl Chloride Monomer (VCM), a topic proposed by INOVYN.

TEACHING METHODS

The Integrated Project is supervised by a whole teaching team gathering 7 Professors of the Chemical Engineering and Material Science + Energy Engineering curricula. A teaching assistant is present to support the project logistics (planification of teaching sessions, communication with the students...) but is not involved in the technical supervision. Additionally, a support is provided by the University of Liège's soft skills team, composed of two psychologists with experience in social psychology of groups and organizations.

Teaching methods include a few hours (about 20 hours spread over the year) of theoretical courses with Professors or external experts, but mostly group work by students and face-to-face interactions between a Professor and a sub-group of students. Plenary meetings gathering all student groups and the whole teaching team take place every month to ensure consistency and follow-up on the groups' progress. The respective share of these teaching activities depends on the moment of the

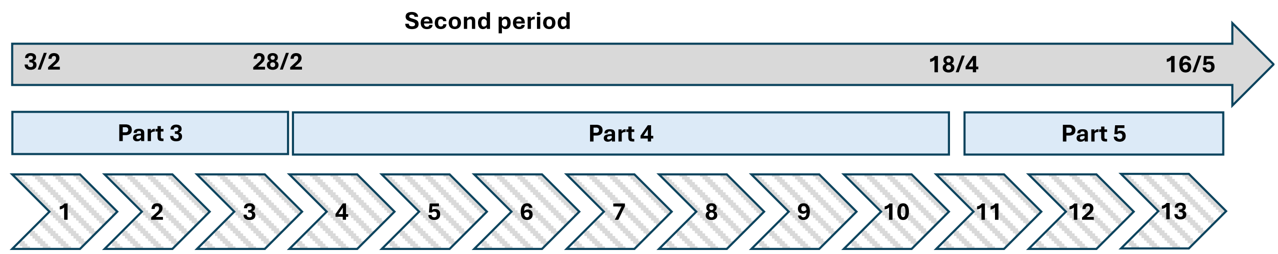

Figure 2: Timeline of the Integrated project at the University of Liège, Spring Semester

year and on the discipline covered at that time. The project is indeed divided into 5 parts, each concluding with a final report and presentation. At the University of Liège, an academic year consists of two semesters (two periods) of 13 weeks of classes, each followed by an exam session. The first semester starts on September 15th, and the second on February 3rd. The distribution of the different parts is presented in Figures 1 & 2.

Part 1: Individual Work

Individual Work on Mass Balances and Literature Reviews

In the first phase of the Integrated Project, students engage in individual work focusing successively on mass balances and literature review. This phase aims to establish a solid foundation for the subsequent stages of the project and individual deliverables (reports) are expected so that each student has to commit from the very beginning. Each student is indeed responsible for conducting a comprehensive mass balance for the synthesis of Vinyl Chloride Monomer (VCM), ensuring a thorough understanding of the material inputs and outputs involved in the process. Additionally, each student performs a detailed literature review to gather relevant information on the chemical and process engineering aspects of VCM production. This includes reviewing existing technologies, process conditions, and recent advancements in the field. The mass balance analysis as well as the literature review last respectively about 1 and 2 weeks.

Consolidation of results and project planning

Following the individual efforts, students consolidate their findings in group sessions. These collaborative meetings are designed to integrate individual results, allowing for the identification of common themes and discrepancies. The groups then plan the next steps of the project, setting clear objectives and timelines. This phase lasts about 1 week and culminates in a presentation where students showcase their mass balance results, literature review insights, and initial process design concepts. This structured approach ensures that all participants have a robust understanding of the project's foundational elements before progressing to more complex modeling and integration tasks.

Part 2: Detailed Models for Thermodynamics, Process Techno-Economics, Kinetics, Reactors, Separation, and Unit Operations

In the second phase of the Integrated Project, students focus on developing detailed models for key unit operations, including thermodynamics, reaction kinetics, and separation processes. This phase is crucial for understanding the fundamental aspects of the process and preparing for the integration phase.

From this second part onwards, students will freely divide into 3 different sub-groups, each of them being followed-up by a Professor:

- Thermodynamics, energy balances and process costing,
- Kinetics and Reaction Engineering
- Separation and Unit Operations

Each sub-group is responsible for a part of the project but of course, close interactions between the subgroups are necessary for the successful completion of the tasks. Regular progress reports presentations (about every 2-3 weeks) are made to share the results with the teaching team.

Thermodynamics, energy balances and process costing: Students begin by selecting appropriate thermodynamic models to describe the behavior of pure components and mixtures within the process operating ranges. They evaluate properties such as density, heat capacity, enthalpy, and vapor pressure. The selection of thermodynamic methods for real systems involves comparing real solution properties to ideal solutions and discussing the differences. Validation of these models is essential, requiring consistency checks based on thermodynamic relations and comparison with at least one other data source. Relevant phase equilibria for pure components and mixtures are characterized, and appropriate thermodynamic models are selected and validated with experimental data. Students also perform initial energy balances and evaluate the rough profitability of the process, creating a proper Process Flow Diagram (PFD).

Kinetics and Reaction Engineering: This section involves determining kinetic laws and mechanisms, selecting catalysts, and designing reactors. Students explore kinetic laws and parameters available in the literature. They propose reaction mechanisms that align with suggested reaction rate laws and demonstrate these laws, explaining any simplifications made. The design and modeling of reactors are performed using Matlab or Python, where students establish mass and energy balances, compute concentration and temperature profiles, and evaluate yield and selectivity. Heat exchange is also considered, usually initiated by a comparison between isothermal and adiabatic approaches and followed by making the link with the types of reactors identified in the literature or from discussion with the industry.

Separation and Unit Operations: Students design and model separation equipment and heat exchangers. They define the separation tasks, including flow rates, compositions, and conditions like pressure and temperature limits. Using first short cut equations, then McCabe-Thiele diagrams, students determine the required number of theoretical stages and design the height and diameter of columns. They also model and size heat exchangers, considering constraints such as volume, length, pressure drop, and velocity. Preliminary designs are rated using methods like Kern and Bell-Delaware, and the results are compared to ensure accuracy.

Part 3: Sensitivity Studies and Model Validation

In the third phase, students focus on performing sensitivity studies and validating the models developed in Part 2. This phase aims to refine the process models and ensure their robustness by evaluating the impact of key process parameters. Moreover, from a soft skills point of view, it is noted that the sub-groups are modified between phase 2 and phase 3 in line with what was announced to students at the beginning of the project. Each student is required to change topics and work with different team members, ensuring a comprehensive understanding of the entire process. This change of sub-groups has several objectives. First, it is intended to foster the acquisition of new technical skills (it is not wished to form specialists in one single discipline in this course). Second, this enhances knowledge transfer as students know from Part 2 that the model they develop will be then used by others in Part 3, and it forces them to keep all other students continuously informed about their choices and difficulties. Finally, it helps developing critical thinking as students in Part 3 have to validate the assumptions and results reached by their peers in Part 2.

Thermodynamics, energy balances and process costing: if needed, students refine their thermodynamic models by validating the models against additional data sources and ensuring consistency with thermodynamic principles. Moreover, they gather the inputs from all subgroups into the process flow diagram that they then use to refine energy balance and profitability estimates performed in Part 2. This task also comes with the first steps towards process design optimization.

Kinetics and Reaction Engineering: In this phase, sensitivity analyses are conducted to optimize reactor performance, considering factors such as feed composition and operating conditions. This involves software tools like Matlab or Python to simulate scenarios and optimize the reactor design. Students also validate their kinetic models and have to identify potential mass and heat transfer limitations related to their choice of catalyst. This step is crucial for ensuring that the kinetic models are reliable and can later be used for process optimization.

Separation and Unit Operations: Students conduct sensitivity studies on the separation processes and unit operations designed in Part 2. They evaluate the impact of variations in flow rates, compositions, and operating conditions on the performance of separation equipment and heat exchangers. This involves using tools like Aspen Plus or Aspen Exchanger Design and Rating (EDR) to simulate different scenarios and optimize the design. Students validate their models by comparing the results with experimental data from the literature and ensuring that the assumptions made in the design are reasonable. This step helps to identify the most critical parameters and optimize the separation processes for better performance and cost efficiency. For the rating of the heat exchanger design, the work is supported by a professor from the energy engineering program, which is very instructive as it forces chemical engineering students to interact with non-chemical engineers.

Part 4: Process Integration

In the fourth phase, students focus on integrating the various components of the process into a cohesive and optimized global flowsheet in Aspen Plus. This phase is critical for ensuring that all elements of the process work together efficiently and effectively.

Global Process Flowsheet: Students begin by combining the sub-models developed in previous parts into a comprehensive global process flowsheet in Aspen Plus. This involves refining the models and identifying key variables that impact the overall process performance. The goal is to create a detailed and accurate representation of the entire VCM production process.

Optimization of Process Operating Conditions: Students work towards optimizing the process operating conditions to enhance efficiency and reduce costs. This includes topological optimization, where the layout of the process is adjusted for optimal performance, and parameter optimization, where specific operating conditions are fine-tuned. Techniques such as pinch analysis are applied for heat integration, ensuring that energy usage is minimized, and heat recovery is maximized.

Cost Evaluation: A detailed cost evaluation of the process is conducted, building on the initial assessments made in previous parts. Students analyze both capital expenditures (CAPEX) and operating expenses (OPEX) to determine the overall economic feasibility of the VCM production process. They also need to come up with a first cash flow diagram of the process that will be used to evaluate the impact of CAPEX, utilities, raw material and product price, process performances... on profitability.

Environmental Impact and Life Cycle Assessment (LCA): Students develop a life cycle thinking approach to assess the environmental impact of the VCM production process. This includes evaluating the process from a cradle-to-grave perspective, considering factors such as raw material extraction, production, usage, and disposal. The goal is not to perform a full LCA, but to identify opportunities for reducing the environmental footprint and improving the sustainability of the process.

Literature Review: An extended literature review is initiated again, now to compare the results obtained from the process models with existing data in the literature. This helps validate the efficiency and effectiveness of their VCM production process. Key Process Indicators (KPIs) such as t_{CO2}/t_{VCM}, kWh/t_{VCM}, and t_{Cl2}/t_{VCM} are used for ease of comparison. Students also identify technological alternatives and potential improvements to the process, considering factors such as raw material efficiency, energy consumption, and environmental impact.

Part 5: Report to a General Audience

In the fifth and final phase of the Integrated Project, students focus on summarizing their work and presenting it to a broader audience. This phase involves updating and validating the project's results, concluding the extended literature review, and considering the broader societal implications of the VCM production process. Regarding this last point, students consider a broader societal overview, assessing the environmental footprint, costs, raw materials use, safety, market conditions, recyclability, toxicity and alternative manufacturing pathways and product replacement solutions. This holistic approach ensures that the VCM production process is evaluated not only from a technical perspective but also in terms of its societal and environmental impact.

The final report is concise, limited to 15 pages and written in the form of a journal article for online publication (see results of the five previous years, [5]). It describes the context of the project and the technical challenge, presents a summary of the main technical results, and validates these results by comparing them to the literature. The report also includes the results of the cost evaluation and the LCA approach. It is designed to be understandable for external readers with a background in chemical engineering. A few days after report submission, students then present their findings in front of the Chemical Engineering Department of ULiège and external experts. The presentation needs to be professional yet engaging, with a maximum duration of 30 minutes per group. The presentation slides are reviewed in advance by the industrial partner to ensure that no confidential information is divulged. An industrial agreement is also required before publishing the project's final article.

Students are encouraged to present results clearly, with enough details, and discuss their impacts critically. They are reminded to follow communication guidelines for both the report and presentation, ensuring that their work is well-documented and easily understandable.

SOFT SKILLS DEVELOPMENT

Additional Lectures

Several "theoretical" lectures are given to students throughout the year. These lectures are either technical and aim to transfer the knowledge needed to solve the technical tasks of the project or dedicated to learning soft skills or reflection. All courses are given by a lecturer specialized in the field. Some courses are also attended by energy engineering students, enriching discussions by bringing together students from different backgrounds.

The first type of course includes process design theory (hierarchical approach), economic evaluation, heat exchanger design and introduction to LCA. These technical skills are not yet mastered by students in their first year of the master's program, but they are necessary to successfully complete the integrated project.

Other courses are also given, linked to the development of non-technical skills such as literature research or scientific writing and presentation. At the start of the project, a lecture is also given on Fermi's questions, where students learn how to solve problems by focusing on orders of magnitude as a first approach. During the fourth part of the project, when the students already have an overview of the process and are integrating all parts into a single flowsheet, an experienced chemical engineer gives a presentation on industrial project management. This session is particularly appreciated by the students, as it enables them to have a very fruitful exchange with a professional about industrial work. The final sessions organized as part of the project are two discussions on ethics and sustainability, led by ULiège's SPIRAL group. The aim of these two sessions is to raise questions and encourage dialogue and reflection on less technical subjects that are also essential for the future chemical engineers taking part in the project.

A visit to the industrial partner's production plant is also planned, usually in Spring. This visit enables students to see the equipment they have designed over the course of the year in real-life conditions, and to observe how the chemical plant operates. The visit is also an opportunity to talk to industrial partners, and to get a better idea of the day-to-day operation of the process, which the students did not necessarily consider during process design. The visit usually lasts a day, enabling the process to be studied in detail and showing students what working in industrial companies is really looking like.

Group Sessions with ULiège Soft Skills Team

During the year, students are supervised by the ULiège Soft Skills team. As said, this team is made up of two psychologists specialized in group management. At least five sessions are organized over the course of the year, where these specialists present the important concepts of group management, and where students can reflect and discuss about their own group dynamics. Discussion is always encouraged at these sessions, as it helps first to highlight and then to solve any problems that may arise during the year.

At the end of Part 1, the Soft Skills team helps students to build up their sub-groups based on the characteristics of each student. A session is then organized a month later to discuss how the group is functioning and to help students communicate better if necessary. At the end of Part 2, a session is organized during which the students watch the recording of their own presentation, then discuss it with the "soft skills" team and possibly a few teachers. Two further sessions are organized in the second semester, on group communication and problem-solving. At the end of the year, a final debriefing of the project is carried out with the Soft Skills team and the two teachers coordinating the teaching team. On the one hand, this debriefing enables the professors to see what the problems and positive points were, so to improve for the next year, and on the other, it helps students to summarize everything they have learned over the year and realize what their abilities and problems were. This forms a good basis for future group work, which they will most probably have in their careers. The Soft Skills team is also always available during the year to help students with any problems they may have, either as a group or individually.

These sessions are also used to discuss the student's peer-evaluation. Part of the final grade for the project is indeed awarded to this assessment done in groups (for details of the evaluation methods, see [4]). This evaluation is based on a discussion between the students, supervised by the Soft Skills team. A grade is assigned to each student, which is then approved by the whole group. This assessment is new from 2024-2025, and replaces the usual peer assessment that was done by each student individually. The aim here again is to open a discussion on each student's work and contribution to the life of the group, and to discuss each student's contributions and shortcomings to give constructive feedback on his or her contribution to the group's work.

CONCLUSION

The Integrated Project in the Master of Chemical Engineering and Materials Science at the University of Liège offers a unique opportunity for students to develop both technical and soft skills essential for their future careers. By working on industrial case studies, such as the synthesis of Vinyl Chloride Monomer (VCM) this year, students face real-world challenges that prepare them for complex industrial situations. The project emphasizes the integration of chemical engineering disciplines, detailed process modeling and optimization of operating conditions, while considering economic and environmental impacts. Regular interactions with industry and academic experts, along with support from the ULiège Soft Skills Team, ensure comprehensive student development. In conclusion, this rigorous and instructive project is highly valued by students and provides solid preparation for their professional future.

REFERENCES

1. Léonard G., Belboom S., Toye D., Dumont M.-N., Léonard A., Heyen G. Recent Evolutions and Trends in the Use of Computer Aided Chemical Engineering for Educational Purposes at the University of Liège. Comput. Aided Chem. Eng. 40: 2941-2946 (2017) https://doi.org/10.1016/B978-0-444-63965-3.50492-X
2. Lewin D., Kondili E., Cameron I., Léonard G., Mansouri S., Martins F., Ricardez-Sandoval L., Sugiyama H., Zondervan E. Agile process systems engineering education: What to teach, and how to teach. Comp. & Chem. Eng. 170: 108134 (2023) https://doi.org/10.1016/j.compchemeng.2023.108134
3. Lewin D., Adams T., Bongartz D., Léonard G., Mansouri S., Martins F., Mujtaba I., Zondervan E. Teaching Process Design – Quo Vadis? Comput. Aided Chem. Eng. 53: 3505-3510 https://doi.org/10.1016/B978-0-443-28824-1.50585-8
4. University of Liège. Integrated Project course description (2024-2025). https://www.programmes.uliege.be/cocoon/20242025/en/cours/PROJ0012-1.html
5. Chemical Engineering Department, University of Liège. Integrated Project (2024-2025). https://www.chemeng.uliege.be/cms/c_4912130/en/chemeng-integrated-project-m1