Computer-based Chemical Engineering Education for Green and Digital Transformation

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ABSTRACT

This paper examines the current state of green and digital integration in traditional chemical engineering education, focusing on how artificial intelligence (AI) can enhance learning. A review of curricula shows that sustainability principles, such as green chemistry, circular economy, and resource efficiency, are often confined to electives rather than core courses. Likewise, digital skills are introduced at a basic level, with limited exposure to AI, especially machine learning, and advanced process optimization. The paper emphasizes the need for a structured approach to integrating sustainability and digitalization into core subjects, supported by interdisciplinary learning. It also explores AI's role in transforming education, particularly in predictive modeling, process optimization, and adaptive learning. The study provides recommendations for redesigning the traditional chemical engineering curriculum to strengthen green and digital transformation.

Keywords: Education, Artificial Intelligence, Optimization, Green Transition, Digitalization

INTRODUCTION

The mission of chemical engineering higher education, particularly computer-aided chemical engineering, is to equip students with the knowledge and skills they need to drive the green and digital transformation. The EFCE Bologna recommendations emphasize data management and digitalization tools as fundamental components of informatics in the first cycle and place a general focus on digitalization at the second cycle [1].

While chemical engineering programs certainly include elements of green and digital engineering, their systematic integration into core subjects is often implicit, making them less visible to students and industry [2]. In fact, the definition of what 'green content' entails is not precisely established. It can encompass the formal 12 principles of green chemistry [3], the 12 principles of green engineering [4], and the 17 sustainable development goals (SDG) [5], as well as more specific topics such as the circular economy, industrial symbiosis, environmental protection, production technologies with reduced environmental impact, sustainable materials and catalysts and related areas.

The curriculum analysis at our institution shows that only a few green engineering principles, such as

maximizing efficiency and integrating energy flows, are explicitly covered. Others appear indirectly through case studies but lack systematic integration. Digital skills are mostly limited to spreadsheet-based data processing, basic programming, and process simulation and optimization. Green and digital topics are explored more deeply in project work, advanced studies, electives, and final theses.

Artificial Intelligence (AI), a key driver of digitalization, presents an opportunity to enhance both digital and green engineering education. It is already significantly impacting education by transforming teaching methods and driving advancements in chemical engineering curricula, especially in PSE/CAPE related courses. However, the interdisciplinary complexity of AI poses challenges, as students need a solid foundation in programming, data science, and statistics, and more importantly, they should acquire skills for the right comprehension and interpretation of solutions they obtained using AI tools. For effective integration, AI should be introduced gradually [6], balancing technical skills with critical thinking, creativity, and ethical awareness while maintaining core engineering fundamentals.

This article examines the readiness of higher education institutions to equip chemical engineering

students for the digital and green transition, along with the challenges they face and the strategies they employ to address them.

CHALLENGES AND CONCEPTS FOR GREEN AND DIGITAL TRANSFORMATION

The main challenge of our society is how to efficiently and effectively address severe global issues—population growth, depletion of non-renewable resources, and environmental and societal degradation. The community strives for sustainable development in general, with a particular focus on sustainable chemical and biochemical industries. To reverse the negative climate trends, the European Commission launched the European Green Deal in 2020 [7] and initiated the foundation of the European Climate Pact [8], with the main goal of making the EU climate-neutral by 2050. Probably the two main related topics are green and digital transformations, which are happening in the EU at an increasing pace, demanding faster and faster economic, social, and personal adaptation. This brings a need for the continuous refinement of the education system, focused on more efficient teaching methods and the introduction of relevant topics and outcomes that students should acquire to be able to face current and future professional challenges.

At the level of the European Federation of Chemical Engineering (EFCE), this transformation is managed through 20 working parties (WPs). The Education WP is primarily focused on teaching methods, topics, and outcomes, while the CAPE WP concentrates on the development and application of process systems engineering (PSE) concepts, algorithms, modelling, and tools. Additionally, there are seven sections, with the Energy and Sustainability section predominantly focused on green transformation.

To cope with current challenges and needs, EFCE recently issued a renewed recommendations for chemical engineering study programs, the EFCE Bologna Recommendations 2020 [1], which can serve as a guide for developing new or adapting current study programs. It can also be used by professionals to assess their missing knowledge and skills, helping them identify areas for their supplementary lifelong learning.

The programming outcomes follow an arrangement introduced by the EUR-ACE® Framework Standards [9], from knowledge to understanding, engineering analysis, engineering design, investigations, engineering practice, making judgements, communication and team-working, and lifelong learning, structured hierarchically over the first and second cycles by applying Bloom's taxonomies. As the first cycle typically provides students with basic knowledge and skills, the first four taxonomy levels are predominantly in place—knowledge, comprehension,

application, and analysis. The second cycle aims to deepen knowledge and skills by incorporating synthesis and evaluation. At the doctoral (third) cycle, it is evident that the highest levels should be applied, enabling students to develop new knowledge and innovative skills for novel engineering applications or enhancing existing ones.

The traditional basic structure of higher education chemical engineering core curriculum [10] is sketch on Figure 1 in black colour. It starts with fundamentals of science and natural sciences like mathematics, physics and chemistry, continuous with engineering fundamentals based on mass and energy balances, transport phenomena as well as separation and reaction engineering and process control. At the second cycle, a process systems approach is introduced, with the primary learning outcome being the synthesis of knowledge in subjects such as process design, dynamics and optimization, culminating in the student project course. The doctoral level is dedicated to generating new knowledge through the application and advancement of cutting-edge methods, as well as the development of novel approaches based on computer-based chemical engineering.

Green, sustainability, and circularity, also regenerative principles related to chemical engineering study programs, are listed together with the four basic components and five branches of AI in Table 1. The reader can find a more detailed description and explanation in the given references. The challenge is how to integrate the principles and AI components into chemical engineering study programs and to what extent. Some principles are simple, others complex, and all interrelated, with varying complexity across AI components. For teaching and study, they should be hierarchically classified using Bloom's taxonomies.

INTEGRATING GREEN AND DIGITAL TRANSFORMATION IN CHEMICAL ENGINEERING EDUCATION

Transforming the traditional chemical engineering curriculum to equip graduates for the demands of a green, digital, and resilient economy is a critical challenge. Larger universities with substantial student populations have addressed this by establishing specialized programs or modules such as Data Science in Chemical Engineering (Purdue), Machine Learning in Process Engineering (Imperial College), Chemical and Biochemical Engineering (DTU) to mention just a few. They pilot AI-driven projects, including digital twins for process control, machine learning for experiment optimization, neural networks for predicting thermodynamic properties, among others. Smaller institutions, meanwhile, must integrate these topics into existing courses.
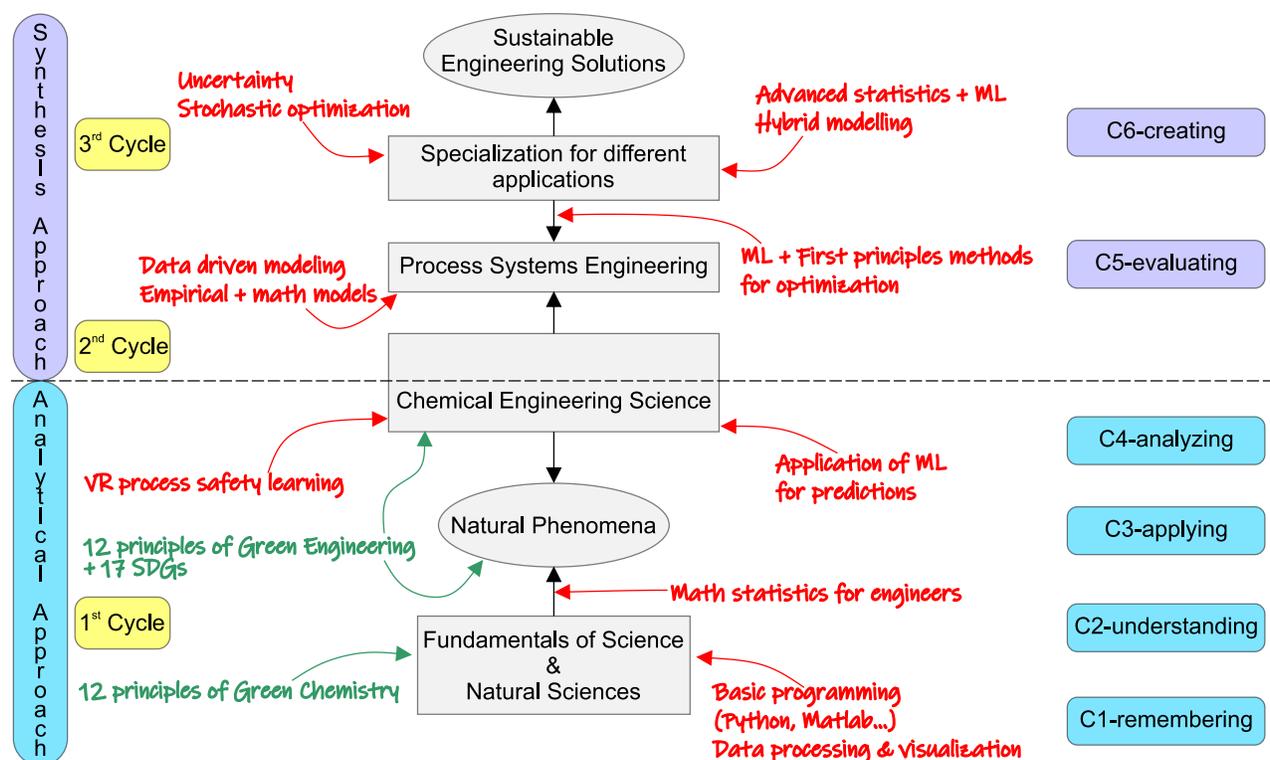
Figure 1: Traditional chemical engineering core curriculum (black), upgraded for green (green) and digital transformation (red). Bloom's taxonomy: Analytical Approach (C1-C4), Synthesis Approach (C5-C6)

Table 1: Green, sustainability and circularity principles, and basic components and branches of AI

Principles of green chemistry [3]	i) Prevention, ii) atom economy, iii) less hazardous chemical syntheses, iv) designing safer chemicals, v) safer solvents and auxiliaries, vi) design for energy efficiency, vii) use of renewable feedstocks, viii) reduce derivatives, ix) catalysis, x) design for degradation, xi) real-time analysis for pollution prevention, xii) inherently safer chemistry for accident prevention
Principles of green engineering [4]	i) Inherent rather than circumstantial, ii) prevention instead of treatment, iii) design for separation, iv) maximize efficiency, v) output-pulled versus input-pushed, vi) conserve complexity, vii) durability rather than immortality, viii) meet need, minimize excess, ix) minimize material diversity, x) integrate material and energy flows, xi)design for commercial "afterlife", xii) renewable rather than depleting
Engineering sustainability principles [11,12]	i) Contribute to building a sustainable society, present and future, ii) apply professional and responsible judgement and take a leadership role, iii) do more than just comply with legislation and codes, iv) use resources efficiently and effectively, v) seek multiple views to solve sustainability challenges, and vi) manage risk to minimise adverse impact to people or the environment.
Core circularity principles [13]	i) Eliminate waste and pollution, ii) circulate products and materials, and iii) regenerate nature
Basic AI components and branches [14]	*Components*: i) learning, ii) reasoning and decision making, iii) problem solving and iv) perception *Branches*: i) machine learning, ii) deep learning, iii) natural language processing, iv) robotics and v) fuzzy logic

Several decades ago, bioengineering and other life science related courses, such as biochemistry, biotechnology, bioreaction engineering, biocatalysis, microbiology, genetic engineering etc., were thoroughly integrated into traditional chemical engineering curricula. However, green content remains largely absent in core courses like transport phenomena, materials, process design, control, and optimization. Illustrative examples in these areas continue to focus predominantly on base industries, which are largely fossil-based.

Digitalization in curricula has been limited to basic tools, such as spreadsheets, introductory programming, process simulation or optimization based on first-principles models using software like Aspen or GAMS. Basic

statistical concepts, including hypothesis testing, receive little attention. Topics like artificial intelligence and its subsets (e.g., machine learning, digital twins) are almost entirely absent at the first and second levels. The same applies to other emerging technologies, such as the Internet of Things (IoT) and blockchain, except for the occasional use of generative AI for text writing. Topics like environmental protection, sustainable development, and the circular economy are primarily confined to elective courses, student projects, and final theses.

The foundational textbooks for chemical and process systems engineering, primarily written in the 1970s and 1980s, remain staples in chemical engineering education, while those on the green transition and digitalization are scarce. This lack of resources has slowed the integration of these emerging topics into curricula. Meanwhile, the shift from traditional textbooks to digital learning platforms for self-paced learning of digital content is becoming increasingly evident.

Group of experts identified key areas for integrating machine learning into research and industry, including materials and catalyst design, industrial analysis, process dynamics and control, and optimization [15]. The challenge lies in selecting suitable courses and defining graduates' roles, whether as users or developers of machine learning tools. Given the field's interdisciplinary nature, they must master both traditional engineering principles and essential digital skills for the future [16].

To tackle these challenges, we present examples of how green chemical engineering and digitalization can be integrated both vertically and horizontally into selected traditional courses (green and red in Figure 1), aligning with key topics from the EFCE Bologna Recommendations [1]. This list is not exhaustive; the examples serve as initial suggestions, and we encourage readers to contribute ideas to enrich the discussion. We advocate integrating the proposed topics into existing subjects instead of adding numerous new courses, as shown in the following examples. A modular approach with pilot projects, electives, and project-based learning allows a gradual transition without overwhelming faculty and students.

Fundamentals of science and natural sciences

Chemistry, physics, and bio-courses should explicitly incorporate all 12 principles of green chemistry into the curriculum, ensuring their clear visibility and practical applications.

Computer programming should include an introduction to a general-purpose programming language, e.g. Python, computing platform, e.g. MATLAB, and preferably also modelling environment, e.g. GAMS along with fundamental libraries for data visualization. It should also cover basic machine learning models, such as linear regression and decision trees, with applications in engineering problem-solving.

Mathematical statistics for engineers should cover hypothesis testing, regression analysis, statistical inference, and data analysis for process monitoring and optimization.

Chemical engineering fundamentals

These courses need to identify ways to explicitly emphasize the 12 principles of green engineering, the 17 SDGs, as well as more advanced principles of circular, restorative and regenerative economics.

Process balances should incorporate the visualization of mass and material flows using modern tools like Sankey diagrams. It should also include the formulation of mass balances for recycling and material reuse processes, emphasizing closed-loop systems and minimizing material losses.

Heat and mass transfer should focus on developing predictive models to evaluate efficiency, integrating experimental data with machine learning algorithms. It should include, for example, the use of recycled insulation materials, supported by case studies on energy efficiency improvements. Additionally, it should explore waste heat recovery technologies in industrial settings.

Thermodynamics should incorporate the application of machine learning for predicting thermodynamic properties of fluids, phase equilibria, and chemical reaction equilibria. It should also integrate data-driven models with classical thermodynamic equations of state to enhance prediction accuracy.

Separation processes should incorporate the use of digital twins to simulate and optimize distillation, absorption, and extraction processes. It should also include case studies on energy-efficient separation techniques.

Reaction engineering should include the prediction of reaction kinetics based on experimental data using data-driven models. It could also integrate advanced algorithms to optimize reactor design and operational conditions, with a focus on sustainable reaction pathways.

Core chemical engineering applications

Chemical process safety could integrate operator training in virtual reality (VR), root-cause analysis to enhance emergency response planning and risk mitigation, and blockchain for secure data management, compliance tracking, and supply chain transparency.

Process optimization for chemical engineering at first cycle should include not only single-objective linear and nonlinear optimization but also statistical analysis, multivariate analysis, multi-objective optimization, and data-driven modeling of complex phenomena and units. It could introduce the integration of such empirical models with mathematical models to improve process efficiency.

Process systems engineering

Process dynamics should encompass mechanistic,

data-driven, and hybrid models, considering both continuous and discrete data due to digitalization. Analysis can be performed using dynamic simulators, computing platforms (e.g., MATLAB, Mathematica), or general-purpose languages like Python. From a control perspective, classical linear controllers, model-based approaches, and AI-driven strategies for nonlinear control should be explored. Additionally, machine learning can enhance adaptive control, real-time fault detection, predictive maintenance, and forecasting.

Process design could incorporate machine learning for selecting optimal process flowsheets, including tools for generating alternative solutions that minimize waste and energy consumption. It should also emphasize life cycle assessment (LCA) to evaluate the environmental impact of different design options.

Advanced process optimization should encompass mixed-integer linear and nonlinear programming, integrating first-principle models with machine learning models to enhance predictive capabilities. It should incorporate multi-objective optimization techniques linking statistical techniques with process optimization for sustainable and efficient system design. The PhD level could explore stochastic optimization methods that incorporate uncertainty quantification and probabilistic modeling.

PERSPECTIVES AND CHALLENGES OF ARTIFICIAL INTELLIGENCE IN CHEMICAL ENGINEERING EDUCATION

Artificial intelligence (AI) is transforming industry and academia, making its integration into chemical engineering education essential. Tailored approaches for undergraduate and graduate programs maximize the potential of AI while addressing the specific challenges.

At the undergraduate level, the introduction of AI tools can enhance fundamental chemical engineering subjects such as thermodynamics, reaction engineering and process control. The benefits of integrating AI at this stage are many. Students are exposed to cutting-edge technologies early on, which improves their problem-solving skills and prepares them for the demands of industry. In addition, AI can personalize learning through adaptive educational platforms and allow students to address their weaknesses in core subjects. However, challenges include the steep learning curve of AI tools and the risk of students relying too much on algorithms without grasping the underlying principles of chemical engineering. A recent study on implementation of generative artificial intelligence in chemical engineering education [17] clearly indicates that a balance between traditional engineering principles and AI applications is crucial to avoid such pitfalls. For lecturers, the inclusion of AI requires curriculum redesign and professional development to ensure effective teaching. Lecturers need to be able to handle AI tools themselves and contextualize their applications in chemical engineering. This increases their workload but also provides opportunities for collaborative research with students on AI-driven projects, which encourages academic innovation.

At the graduate level, AI can drive specialized research and innovation. Advanced topics such as data-driven modeling, optimization, and predictive maintenance can be integrated into courses. The benefits of AI at the graduate level go beyond skill development and also foster interdisciplinary collaboration. Graduate students can work at the intersection of AI, chemistry and engineering, exploring novel solutions to industry challenges. However, there are still pitfalls, such as the possibility of over-fitting models or misinterpreting AI-generated results due to an insufficient understanding of the principles of data science. This requires a solid foundation in statistics and programming, which may require additional courses or self-directed learning. For educators, integrating AI at the graduate level provides an opportunity to advance their research agendas and obtain funding in emerging fields. However, it also requires significant effort to keep pace with rapidly evolving AI technologies and their applications. Collaboration between faculty in chemical engineering, computer science and data science departments can alleviate some of these challenges and promote a holistic approach to AI education.

Looking to the future, the role of AI in chemical engineering education is poised to grow. Advances in generative AI, real-time data analytics, and digital twins will continue to transform the curriculum. Students will be able to interact with AI tutors, design processes in virtual environments and contribute to AI-powered research projects. While these developments are very promising, ethical considerations, such as data privacy and algorithmic bias, must be carefully considered. It is clear that integrating AI into the chemical engineering curriculum represents both a challenge and an opportunity. By thoughtfully incorporating AI tools into the undergraduate and graduate curriculum, educational institutions can prepare their students to lead and shape the future of chemical engineering and raise a generation of engineers who are not only technically proficient, but also adaptable and innovative.

It is not difficult to imagine all the benefits that digitalization and artificial intelligence will bring to the learning processes in chemical engineering. From the students' perspective, these will certainly include personalized learning with an increasing presence of virtual reality. This ranges from digital twins of the phenomena and processes studied to digital twins of entire courses and eventually even the lecturers — why not? From the lecturers' perspective, before we are replaced by digital twins, AI will enable data-driven curriculum

improvements, advanced teaching materials with virtual and augmented reality demonstrations, early warning systems to detect student learning difficulties, and curriculum progress tracking, among other things.

However, it is important to emphasize that due to digitalization and/or artificial intelligence, it will be crucial for chemical engineering students to acquire sound skills in data processing (e.g. data mining, data crunching and pre-processing, understanding data bias and variability, feature engineering, ethical and legal considerations, etc.) as well as in processing, analysis and, most importantly, in assessing the validity and significance of the results obtained.

CONCLUSION

This study highlights the lag in integrating green and digital competencies into the core chemical engineering courses. Systematic teaching materials, both traditional and digital, are essential for educators and students. As a novel approach, we propose the incorporation of green and digital content across the entire vertical structure of chemical engineering education, aligned with EFCE Bologna recommendations—spanning from fundamental sciences through chemical engineering principles to process systems engineering. To support this transition, we encourage the development of common guidelines, e.g. by EFCE, EURECHA or other professional associations, enriched with clear instructions for embedding green and digital competencies into chemical engineering curricula, equipping future engineers with the necessary skills to drive sustainable and digital transformation.

ACKNOWLEDGMENT

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