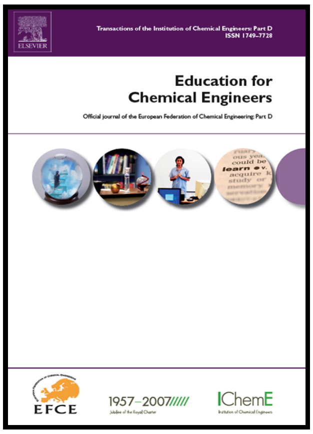
Journal Pre-proof



Digital Tools in Chemical Engineering Education: the needs and the desires

Isuru A. Udugama, Martin Atkins, Christoph Bayer, James Carson, Duygu Dikicioglu, Krist V. Gernaey, Jarka Glassey, Mathew Taylor, Brent R. Young

PII: S1749-7728(23)00019-2

DOI: https://doi.org/10.1016/j.ece.2023.05.002

Reference: ECE382

To appear in: *Education for Chemical Engineers*

Received date: 2 May 2023
Accepted date: 9 May 2023

Please cite this article as: Isuru A. Udugama, Martin Atkins, Christoph Bayer, James Carson, Duygu Dikicioglu, Krist V. Gernaey, Jarka Glassey, Mathew Taylor and Brent R. Young, Digital Tools in Chemical Engineering Education: the needs and the desires, *Education for Chemical Engineers,* (2023) doi:https://doi.org/10.1016/j.ece.2023.05.002

Digital Tools in Chemical Engineering Education: the needs and the desires

Isuru A. Udugama[1,*], Martin Atkins[1], Christoph Bayer[2], James Carson[1], Duygu Dikicioglu[3], Krist V. Gernaey[4], Jarka Glassey[5], Mathew Taylor[1], Brent R. Young[6]

[1] Ahuora – Centre for Smart Energy Systems, School of Engineering, University of Waikato, Hamilton, 3240, NewZealand
[2] Department of Process Engineering, TH Nürnberg, Nürnberg, 90489, Germany
[3]The Advanced Centre for Biochemical Engineering, Department of Biochemical Engineering, University College London, London WC1E 6BT, United Kingdom
[4]PROSYS Research Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Søltofts Plads, Building 228A, Kgs. Lyngby 2800, Denmark
[5]School of Engineering, Merz Court, Newcastle University, Newcastle upon Tyne, NE1 7RU United Kingdom
[6]Department of Chemical and Materials Engineering, University of Auckland, Private Bag 92019, Auckland, New Zealand
*isuru.udugama@waikato.ac.nz

Abstract

Educators in chemical engineering have a long and rich history of employing digital tools to solve fundamental engineering problems. Today, with the megatrend of digitalisation, there is a growing set of tools that can be used for chemical engineering education. However, identifying which tool is ideally suited to support teaching a given chemical engineering concept can be challenging. To answer this question a survey was distributed to Heads of Departments at IChemE institutions and members of the IChemE committees focused on digitalisation. The survey respondents rated Microsoft Excel (VBA), commercial simulators, and scripting tools as ideal for teaching core subjects such as mass and energy balances, mass transfer and reaction engineering while respondents found 3D Models, and Virtual/Augmented Reality models as being most suited for teaching subjects such as process design, safety and sustainability. Mathematical/programming simplicity, ease of maintenance, and low initial investment costs were identified as key non-technical aspects that will hinder the adoption of a given digital tool. Weighing the benefits of education and non-technical hurdles, the respondents preferred the use of simpler digitalisation platforms such as Excel and scripting languages over the more advanced platforms such as Virtual/Augmented Reality where possible. It was identified that the widespread adoption of more advanced

digitalisation tools will require removal of the above mentioned non-technical barriers as well as other barriers such as tool shareability.

1. Introduction

Digitalisation and Industry 4.0 collectively refer to a paradigm shift in how goods and services are designed, manufactured and serviced across industries. The process engineering profession (encompassing energy, chemicals, food, renewables and biotech) has also been affected by these megatrends with the concepts of Digital Twins and Big Data analytics being identified as two key pillars in delivering changes e.g., (A. Udugama et al., 2021). For educators in the process engineering field these changes raise the following two questions.

1) How can digital tools be used in chemical engineering education? For instance, using software to illustrate essential concepts, e.g. set up of balance equations
2) What should be taught in a chemical engineering curriculum, such that graduates are able to develop the next generation of digitalisation solutions? For instance, developing digital models to track vital state variables in a plant. E.g, for the prediction of hard to measure variables such as critical quality attributes (Li et al., 2021)

Both of the above questions are worthy of deeper investigation and are to some degree intertwined. Currently, the Education Special Interest Group (EdSIG) of the Institution of Chemical Engineers (IChemE), which comprises both academic and industrial practitioners are discussing these two questions in detail. The objective of EdSIG is to "further information exchange between universities and industry, develop a network of interested and committed chemical engineers, and share expertise and ideas for best practice in chemical engineering education.". Currently, EdSIG is developing recommendations on how digitalisation should be incorporated into the chemical engineering curriculum. These recommendations together with input from other relevant committees, (e.g, Digitalisation Technical Advisory Group (DigiTAG)) will form the basis of future IChemE guidelines (and examples) for incorporating digitalisation concepts at accredited institutions.

Looking for answers to the question “what should be in the chemical engineering curriculum?” (Udugama et al., 2022), three surveys centered around the University of Auckland, an IChemE accredited university program were conducted. The surveys were directed to alumni from the Department of Chemical and Materials Engineering at the University of Auckland, international experts in digitalisation technologies in both academia and industry, and the academic staff at the department. The surveys were able to pinpoint industrial needs, best practices and practical limitations to be considered for digitisation in the chemical engineering curriculum. Based on these considerations, a hybrid approach of embedding digitalisation concepts into existing courses and developing standalone courses was proposed. With the proliferation of digitalisation tools in the domain of chemical engineering, there is a need to identify the state-of-art solutions that are at the disposal of a chemical engineering educator. In (Zandi, Glassey and Young, 2022) the authors also identified this need and conducted a high level survey which illustrated a clear need to incorporate digitalisation tools into chemical engineering education. These tools must be reconciled with practical needs, desires and limitations of teaching core subjects in chemical engineering.

The focus of this manuscript is on answering the question “how can digitalisation be used in chemical engineering education to enhance student learning by supporting teaching of core concepts?". To address this a literature review is conducted to establish the state-of-art the digitalisation tools and categorise them into broad technologies that span from excel based tools to augmented reality. A targeted survey is then conducted to identify educational benefits, economics, and practical limitations of these digitalisation tools in teaching specific core chemical engineering subjects. Based on the results of the survey, a set of conclusions are made and the suitability of applying a given type of digitalisation tool to facilitate teaching activities of a given core chemical engineering subject are identified.

2.0 State-of-art

The use of digital tools in chemical engineering education has been a practice for decades. Almost all universities that offer an accredited chemical engineering degree use commercial process simulators in delivering some core courses. For example, (Young, Mahoney and Svrcek, 2001) proposed the use of "real time computer simulation" for teaching chemical engineering undergraduates process control in a hands-on and an intuitive manner. (Luyben, 2006) wrote a text book detailing how distillation design and control can be taught using the commercial simulator ASPEN™ Simulation. Recently (Young, Taube and Udugama, 2023) introduced a text book detailing a real time computer simulation" for teaching distillation process control to a postgraduate level. (Calvo and Prieto, 2016) reported the use of ASPEN™ simulator to teach advanced distillation principles through a project based learning approach. (Zhang et al., 2013) discussed how open ended commercial simulators were used at the University of Auckland, New Zealand, to teach basic theories of process control and develop an intuitive understanding of process control. It should be noted that these commercial simulators have the ability to provide a flexible platform for developing digital twin technologies, e.g., (Alford et al., 2022).

The use of the scientific programming platform MATLAB in chemical engineering education is also an established practice, although there is a trend toward the use of Python/other free coding languages (as discussed later). (Martín et al., 2011) developed code to teach advanced thermodynamics using MATLAB. Recently, (Udugama et al., 2020) proposed using Simulink together with the Tennessee Eastman process simulation code as a tool for teaching process control. (Sunarso et al., 2020) illustrated how MATLAB was used in project-based assessments related to unit operation modelling at the Swinburne University of Technology Sarawak Campus, Malaysia. (Bequette, 2003) wrote a text book that can be followed by engineering students to use MATLAB™ for process control education. (Gargalo et al., 2022) discussed the need to develop an on-line and open-source educational computer-aided platform/simulator as a part of preparing students for Industry 4.0 applications. (Chaves et al., 2022) presented how the open source metabolic model simulation OPTFLUX can be used as a digital tool in teaching chemical engineers about cell metabolism.

Microsoft Excel and its macro functions have been used extensively as a digital tool in chemical engineering. This includes the development of Excel add-ins to teach engineering thermodynamics (Castier and Amer, 2011). In (Briones and Escola, 2019) the authors present the use of Excel and its built-in Excel solver tool to teach students how heat exchanger networks can be modeled and optimized. In (Wong and Barford, 2010) the authors discuss how Excel and its built in Visual Basic for Application programming can be used as a valuable digitalisation tool for teaching core chemical engineering courses such as modeling a batch reactor. At the University of Waikato, New Zealand, fermentation modelling is taught using Microsoft Excel where students have to set up a relatively complex fermentation model which requires numerical integration.

With the COVID-19 pandemic, the concept of virtual laboratories has become a standard tool that is used by many universities and is likely to be a key tool in delivering a chemical engineering education going forward (Glassey and Magalhães, 2020). The term virtual lab covers a broad spectrum of applications. At its core a virtual lab application consists of a mathematical model (prediction engine) and a graphical user interface. For example,(Selmer et al., 2007) discussed the concept of "WebLabs" as a method for teaching chemical engineering labs online with specific experiences gained by the authors at that time in conducting these type of online labs. (Domingues et al., 2010) developed two virtual laboratories that focused on describing industrial scale fermentation process fundamentals. (Ramírez et al., 2020) developed a virtual lab to support a course on chemical reaction engineering. (Seifan, Robertson and Berenjian, 2020) suggested the use of virtual lab based learning to improve pre-requisite skills for students enrolled in an industrial biotechnology course. (Viitaharju et al., 2021) developed a comprehensive digital laboratory safety training platform called AALTOLAB which consists of an interactive, web-based 360° virtual laboratory, integrated with a Moodle-based digital exam with automatic assessment. The fidelity of the Virtual lab is determined by the underlying mathematical model while the user experience of the model is determined by the user interface, which can be anything from simple graphics to a web-based 360° virtual laboratory. To this end, the classification of virtual labs can also benefit from the concept of "looks like" and "feels like" that was proposed by (Yu et al., 2022) for classifying digital twin technology in the energy space.

Virtual reality (VR), in some way is a natural extension of virtual laboratories, however VR applications use an integrated software and hardware platform that enables the development of an immersive education environment. VR has gained popularity in the recent years, however, the concept of VR was explored by (Norton et al., 2008) some time ago initially, where a real process plant was created on a VR based immersive learning environment and as an aid in teaching process systems engineering concepts. A key benefit of VR in the context of chemical engineering education is its ability to provide a "realistic" platform (Udeozor et al., 2021). This is of particular benefit in exposing students to potentially hazardous operations in the chemical industry (Garcia Fracaro et al., 2021; Toyoda et al., 2021) investigated the socio-economic drivers of getting immersive virtual reality based learning implemented in a chemical engineering context.

In recent times the concept of Augmented Reality (AR) has also been applied in chemical engineering education. For example (Low, Poh and Tang, 2022) developed two interactive AR lessons on centrifugal pumps and shell-and-tube heat exchangers using the commercial VR platform EON-XR. While (Solmaz et al., 2021) assessed the practicality of developing a combined VR and AR teaching tool which included the development of a case study that focused on liquid soap synthesis. (Solmaz et al., 2021) concluded that despite the current advances, the implementation and maintenance of such a combined AR and VR system requires a highly skilled set of individuals.

3.0 Needs and Desires

Both the digitalisation megatrend and the COVID-19 pandemic have resulted in a "proliferation" of digital education tools that can be as simple as an Excel spreadsheet or as complicated as a full virtual reality solution. Some tools are based on custom code written using programming languages such as Python which are supported by the academics who developed the tool, while others come with commercial support.

While academics may keep on exploring and developing different digital tools for education, they should only be introduced in a course/classroom setting

- If there is a direct influence on the quality of teaching
- The students are able to handle the added load associated with learning a new tool.

Digitalisation tools can improve quality of delivery of core material by either replacing the existing practices by moving these concepts into the "digital realm" or by developing new capabilities that will enable educators to either better illustrate a fundamental concept, which would be otherwise difficult or impossible to illustrate or allowing the educators to tackle more complex topics which otherwise would be too complicated to solve by traditional "pen and paper" means. At the same time there are non-technical aspects to consider such as:

- The free accessibility of the tool to an educator: The open-source process simulation software e.g. DWSim, is more accessible than many traditional commercial process simulators as it is free. However, commercial simulators are frequently offered to universities without charge (or for a token payment) for education purposes.
- Development and maintenance: Commercial tools would be the easiest to develop and maintain as there will be dedicated support staff as well as pre-loaded examples which make the use of these tools easier.
- Low to moderate cost of development both in terms of infrastructure and software: For tools using VR and AR the cost of infrastructure needed potentially plays a significant role in their implementation.

To this end, the sustainable adoption of digital tools in the domain of chemical engineering education requires the following core questions to be answered.

- How important are non-technical aspects (like ease of use, maintenance, upfront costs) in ensuring the fuller integration or expansion of digital tools in the chemical engineering curriculum?
- What is the value proposition of each type of digitalisation tool considering its benefits to teaching as well as all non-technical aspects?
- What type of digitisation tool can be used for teaching a given core chemical engineering subject. If so how would/should they be used?

3.1 Digitalisation Survey

In order to answer the above questions, the authors developed the following targeted survey on digitalisation. The survey was then released to the members of DigiTAG and EdSIG groups of IChemE and to the heads of departments of accredited IChemE engineering departments. The responses were recorded anonymously. Table 1 details the questions

Table 1: Digital tools in chemical engineering survey to experts

---

Digital tools in Chemical Engineering Undergraduate Education

Digitalisation and Industry 4.0 collectively refer to a paradigm shift in how goods and services are designed, manufactured and serviced across industries. For educators in the process engineering field these changes raise the following question. HOW CAN DIGITAL TOOLS BE USED IN IMPROVING CHEMICAL ENGINEERING EDUCATION?

Your answers to this survey will help us with understanding the use cases and value of digital engineering education tools out there.

1. What is your current title?
2. In your opinion, how relevant are the following factors when developing digital tools for chemical engineering undergraduate education?
    - Mathematical and programming simplicity
    - "Zero or low" upfront capital cost and licensing fees
    - Ease of maintenance

- Student's familiarity with tool/underlying program

3. Considering non-technical aspects and benefits to teaching, how would you rate the value propositions of the following tools in the context of chemical engineering undergraduate education?
    - Excel based tools
    - Scripting based tools (e.g., Matlab/Python)
    - Commercial Process Simulators
    - Programming Languages (e.g., C++, Java, C#)
    - CAD 3D/P&ID drawing tools
    - Virtual Labs/OTS
    - VR/AR
4. Considering the value proposition, which of the following digitalisation tools would you use to teach which subject?
    - Thermodynamics
    - Mass and energy balances
    - Heat and mass transfer
    - Reaction and fermentation engineering
    - Separation processes
    - Process design
    - Sustainability
    - Process dynamics and control
    - Safety
5. In your opinion, how can the afore-mentioned digital tools help with improving the teaching of each of the subjects discussed? (Please specify which tool(s) you think are best suited to deliver this change).
6. Do you have any other comments you would like to make?

3.2 Survey Results

The survey was answered by 16 respondents (see Figure 1). The majority of respondents identified their current role as an associate professor/reader. Three respondents listed non-academic positions as their current title, these respondents are likely the industrial members of the DigiTAG and EdSig committees. Please note that the authors of this manuscript did not respond to this survey.

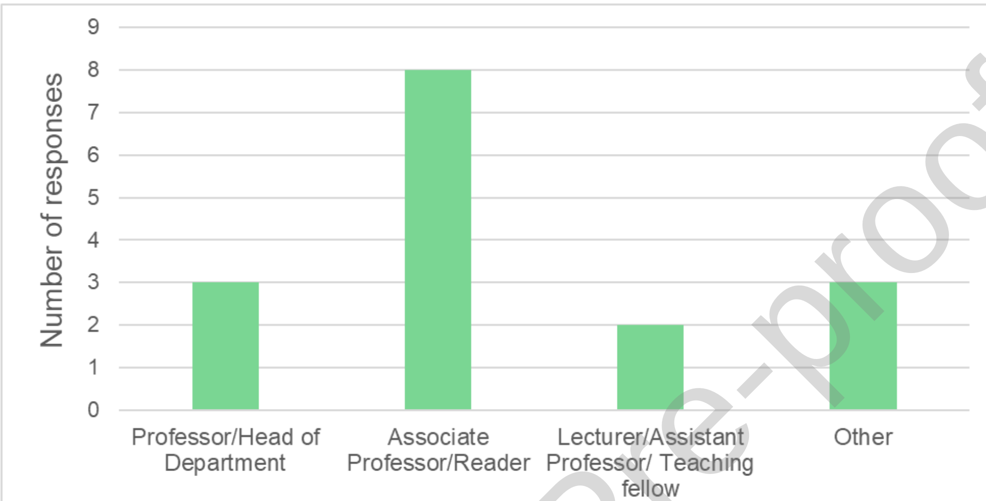


Figure 1: Current role of the respondents to the survey (n=16).

3.2.1 Identifying key non-technical factors

Figure 2 illustrates the opinions of the respondents on the relative importance of key non-technical factors. From analysing Figure 2, it is apparent that all identified factors were deemed to be of importance (important or above) by a great majority of the respondents. Out of the non-technical factors identified, mathematical and programming simplicity seems to be the most important factor that should be considered when developing digital tools for chemical engineering undergraduate education, with all respondents rating this aspect at "important" or above and a great majority rating it as "very important". Considering the supporting role digital tools have in a chemical engineering context, this result is justified, as simplicity in mathematics and programming will enable an educator to focus on using the tool to improve a student's understanding of a core subject rather than on bringing a student "up-to speed" on a complex program. A similar result can also be seen for the aspect of students' familiarity with a tool/underlying program; as a majority of the respondents rated this aspect as "fairly important", though one respondent considered this aspect not important at all. A similar reasoning can be given for this result, as the relative familiarity of students towards a given tool or a program reduces the time an educator needs to spend on explaining its working. However, this means to use tools such as process simulators effectively in the chemical engineering curriculum, upfront time needs to be allocated within the curriculum to bring the students "up-to speed".

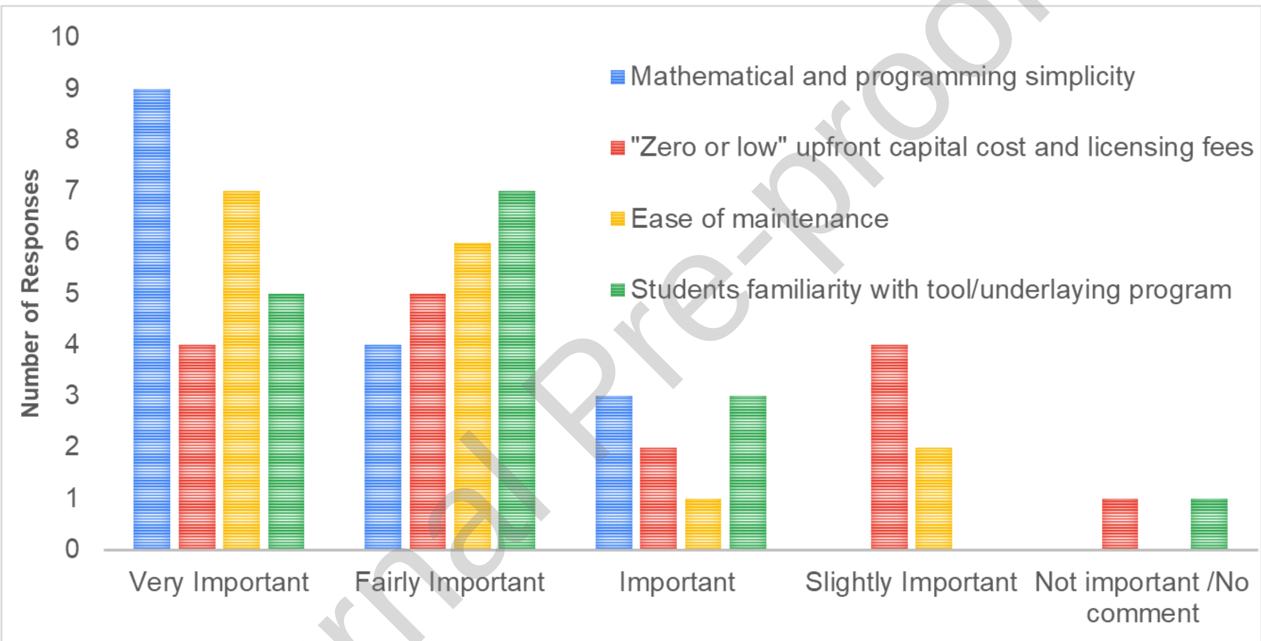


Figure 2: Respondents' opinions on the relevance of key non-technical factors in developing digital tools for chemical engineering undergraduate education (n=16).

Ease of maintenance was identified as another important non-technical factor with the majority of the respondents rating this factor as "fairly important" or above. This response is in-line with the authors' collective experience, where the departure of a key researcher that created a given education digital tool has resulted in the tool being phased out of the curriculum over time. Using commercially developed tools or tools that are supported by a strong development community can mitigate this factor. However, considering that most of the respondents also identify “zero or low” upfront expenses and licensing as an important factor, the use of commercially developed tools can be somewhat difficult to justify, unless they are offered free of charge or at a substantially reduced cost. Although most academic institutions receive commercial software at a reduced licensing price this also means relatively cutting-edge technology with upfront hardware purchases (such as VR) will be difficult to implement.

3.2.2 Value proposition of digitalisation tools

To understand the value propositions of different digitalisation tools that can be used to support chemical engineering undergraduate education, the respondents were asked to rate the usefulness of these tools considering the complexities brought on by the non-technical aspects and their benefits to teaching (Figure 3).

Figure 3 Respondents opinion on the usefulness of different digitalisation tools applicable to chemical engineering undergraduate teaching considering both non-technical aspects and benefits to teaching (n = 16).

From analysing Figure 3, it can be seen that a vast majority of the respondents think Microsoft Excel based tools provide an "excellent" value proposition when it comes to chemical engineering teaching. This result is expected as Excel based tools are likely to have excellent performance in non-technical aspects while also providing a solid and versatile platform for developing digital tools, be it as a simple visualisation tool, optimizer, or a calculator. The students' relative familiarity and likely prior use of Excel is also an added benefit. Commercial process simulators are also seen by most of the respondents to have an "excellent" value proposition. This is likely due to the ease of use, relatively thorough coverage, and the simulator's versatility in setting up and analysing advanced scenarios outweighing the negative non-technical impact needing licensing fees to be paid. Most of the respondents also rated the value proposition of 3D computer-aided design (CAD) and P&ID drawing tools as "very good" or above. CAD and P&ID tools are needed in teaching core process and product design competencies in chemical engineering and are equipped with graphical user interfaces that can be mastered by undergraduate chemical engineering students with some effort.

The majority of respondents also see scripting languages (such as MATLAB and Python) as having a value proposition that is "very good or above". In comparison to the tools mentioned above, these scripting languages require students to spend time and effort in understanding basics of computer programming and are open-ended in nature. However, they provide an excellent and versatile platform to set up multiple types of digital models and consist of inbuilt digital tools that can be configured. A majority of the respondents found programming languages (C, C++) to have a value proposition which is "fair" or below. This is because these languages are much more complicated to write in and require significant time and effort from students to master, while also requiring them to code many of the tools from ground up. As such, the value proposition of pure coding languages in chemical engineering education is somewhat questionable.

The respondents' opinions on the value proposition provided by virtual labs/Operator Trainer Simulators (OTS) and VR/AR was mixed with some finding it to be "excellent" while others found it to be "poor". The reason for this mixed opinion can be relative niche use of these concepts in chemical engineering education. On the one hand, these tools provide an excellent immersive and unique environment for educators to explain complexities of chemical engineering. But on the other hand, these tools require maintenance and notable upfront costs both in terms of capital investment and time. Another factor to consider is the varied quality of the virtual lab/training simulators due to the bespoke nature of these tools, which are often developed by academics.

3.2.3 Matching tools with core subjects

In order to match up the digitalisation tools identified with core chemical engineering subjects the respondents were asked to identify which digitalisation tools they would use to teach a given subject, considering the overall value proposition of the digital tool and the core chemical engineering subject. Figure 4 illustrates the results obtained (note that the respondents could choose multiple digital tool options).

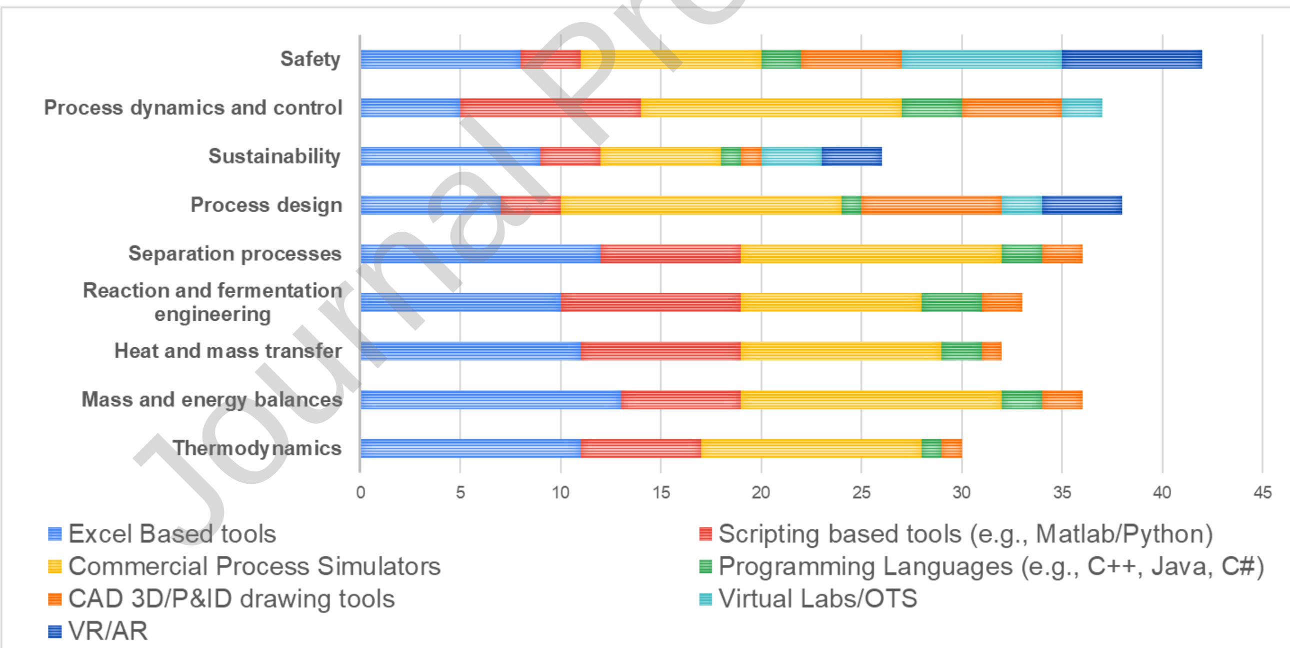


Figure 4: Respondents' opinions the appropriate digitalisation tool to use for given subjects (n = 16).

Figure 4 clearly shows that Excel based tools and commercial process simulators are preferred by respondents over other tools to teach all core chemical engineering subjects. In teaching the fundamental chemical engineering subjects of thermodynamics the respondents prefer to use both Excel tools and commercial process simulators, while a notable portion of respondents also identified scripting-based tools as a potential option. This preference is expected, as Excel tools and scripting languages provide a versatile platform on which calculations and data visualization can be easily performed. One respondent commented "Excel-based. Students can develop calculation procedures by theirself [sic]. Typically, they just need a solver". In comparison, the commercial process simulators come preloaded with key thermodynamic property packages. As one respondent commented "Process simulators can be used to compare different thermodynamic package [sic], understand the phase changes, and equilibrium processes". When analyzing the results for mass and energy balances, a similar preference can be seen. One respondent captured the popularity of both Excel tools and process simulators in in the following comment: "A lot can be taught initially using hand calculations and Excel, but process simulators are really needed for performing plant-wide balances."

In teaching heat and mass transfer, both Excel and commercial process simulators were the choice of the majority while a significant number also identified scripting languages as a tool of relevance. As put by one respondent "For many practical applications Excel is entirely adequate; however, for complex geometries, spatially variable thermal properties and radiation, MATLAB or FEA is required". This shows both the versatility of Excel as well the drawback of using Excel when working with more complex problems. In comparison, the use of a process simulator will likely have the same versatility without any of the drawbacks. As pointed out by another respondent "Flow sheeting simulators are the easiest to work with (as far as the students understand the underlying principles)".

For reaction and fermentation engineering, respondents equally preferred Excel, scripting languages and commercial process simulators. The following comment from a respondent sums up the rationale behind these choices "As it is known, reaction engineering is a field with a focus on mathematics and physics. For this reason, mathematical calculation, simulation, commercialized process simulators will be very useful for learning the subject in a very comprehensive way, especially for reaction engineering". For separation processes, commercial process simulators are the most preferred tools by the respondents. As said by a respondent "Introductory examples can be performed using Excel for a number of units, but for multiple units a process simulator is preferable". A small number of respondents also identified programming languages as a potential tool. This is likely due to the apparent complexity of reaction and fermentation engineering subjects and their use of ordinary and/or partial differential equations.

In teaching process design, process simulators are clearly preferred. For the first time, 3D CAD/P&ID software are also preferred by a significant number of the respondents. Moreover, the use of Virtual Laboratories/OTS and VR/AR are recorded as potential choices by the respondents. As put by one respondent: "Process design is best done with a process simulator", this sentiment is echoed in many chemical engineering departments where a major part of process design is taught with the aid of commercial process simulators. Plant 3D CAD/P&ID software can also be beneficial in getting students oriented with sizing and instrumentation of plants.

In teaching sustainability subjects Excel and process simulators are preferred, while a small number of respondents identified scripting language, Virtual Laboratories/OTS and VR/AR as potential choices. One respondent stated "Excel is enough. When employing life-cycle analysis, another tool can be used." While another stated "Flow sheeting simulators are a good tool". Virtual Laboratories/OTS and VR/AR can potentially be great aids in providing an immersive experience in driving sustainability goals. In teaching process control and dynamics, commercial process simulators were a clear preference followed by scripting languages and then Excel. According to one respondent, "MATLAB/Simulink and process simulators are really needed - there's not that much that can be done in Excel". This comment illustrates a limitation of Excel in supporting complex dynamic process simulations that are often needed for process control, unless one uses VBA extensions.

The use of Virtual Laboratories/OTS and VR/AR as well as process simulators and Excel are all identified as potential preferred choices for teaching process safety by the respondents. It should be noted that this is the only instance where Virtual Laboratories/OTS and VR/AR can be seen as bona fide choices for teaching a core chemical engineering subject. One reason for Virtual Laboratories/OTS being identified as a preferred choice in process safety is the immersive and comprehensive environment these new tools provide as discussed by one of the respondents: “Software with established complete systems/walk-around plant with scenario development and result analysis”.

4.0 Discussion

Chemical engineering as a profession has employed coding languages as the basis for model development for decades, e.g the use of Fortran (Downs and Vogel, 1993). Software platforms such as MATLAB have since been popular while PYTHON is the latest iteration of this trend. While coding skills in these platforms are essential skills for future industrial digitalisation implementation, these should be thought of only as platforms that can be used to develop digitalisation tools for the purpose of chemical engineering education. In other words, Microsoft Excel, MATLAB, Scripting languages and programming languages are platforms that can be used for the purpose of improving chemical engineering education like Process simulators, VR/AR, Virtual Lab/OTS platforms. When analyzing the survey results, some educators are struggling to differentiate the platform role scripting and programming languages can play. As such, the authors would like to reiterate that the objective of this manuscript is to identify how different platforms can be used in digitalisation of chemical engineering education.

However, to use a given platform students require a base competency of formulaic skills, where “programming and algorithmic thinking (and basic engineering logic) should be the first step, to develop adequate digitalisation skills” (as mentioned by one respondent). As such, the level of student’s competency in each platform can dictate the success of using that platform to develop digitalisation tools. As such, there can be a need to shift the curriculum to account for any deficiencies, like in the case of the Department of Chemical Engineering at the University of São Paulo in Brazil (Teles dos Santos et al., 2018).

Taking these factors into consideration it can be clearly seen that educators prefer the use of simpler platforms such as commercial process simulators, scripting languages and Microsoft Excel. Based on the survey evidence the preference is due to a favorable trade-off between the enrichment of the teaching experience and the non-technical complexities that must be overcome when introducing a digitalisation tool into a chemical engineering curriculum, including the familiarity of students with the platform. The educators also tend to discard the development of more complex platforms such as VR/AR and Virtual labs/OTS and the use of programming language as a platform for developing digitalisation tools.

Out of all the platforms, the VR/AR platform is the newest and hence they tend to evolve the fastest. In general, the following positive trends mean that the overall value proposition of the VR/AR platform will continue to improve.

- Development of simple interfaces: Programs such as Unity Virtual Reality Engine and Unreal Engine 4/5 are reducing the upfront effort and maintenance costs of implementing digital education tools on a VR/AR platform. These tools can be programmed by graduate level students without the need for specialists. In the future, further platforms will likely be developed which in the future reduces the impact of the technical barriers.
- Developing an eco-system: Platforms such as GitHub are starting to see a VR/AR community evolving. As such, education tools maybe developed by users as a part of an eco-system. Many VR/AR platform based education digital tool development projects are also explicitly considering maintenance as an explicit part of the projects. For example, having graduate or final year undergraduate student projects that systematically further the capabilities of a given education tool is used as way of ensuring an active eco-system.
- Reduction in hardware prices: For VR/AR platforms, the cost of the hardware is dropping over time. This also reduces the overall cost of incorporating them into a chemical engineering curriculum and often the hardware can be used for multiple purposes.

A key barrier to the wide adoption of an advanced chemical engineering educational digital tools (in all platforms) is the legal barriers to its shareability. Currently, the intellectual property right of an advanced educational digital tool developed in a university environment belongs to that university. However, an advanced educational digital tool developed as a part of a research project might explicitly require the tool to be shareable. On the one hand, from the university's perspective if an advanced educational digital tool is of value to another institute they should pay for the use of that tool. These "fees" can be used for the maintenance and improvement of a digital education tool. For example, the digital educational tool developed in (Udugama et al., 2020), required modification to its code to ensure compatibility with a newer version of the MATLAB platform. On the other hand, as identified by the survey, such upfront and ongoing costs can potentially be a barrier to the adoption of advanced educational tools. As such there is a need to "re-think" strategies with regard to ownership of advanced educational digital tool that are made in a university setting. For example, one could consider moving to a community based model where the advanced educational tools are regularly improved. On the other hand, making the tool freely available can also help with its upkeep. An example there is the suite of benchmarking models that have been developed throughout the years for studying wastewater treatment operations. Many of the tools that have been developed are made available for free via Github (https://github.com/wwtmodels/)

Identifying how digital tools can help with digitalizing current education practices and how digital tools can provide new capabilities that are otherwise not available in the future is another area of interest to streamline the development of advanced educational digital tools. Table 2 shows the combined opinion of respondents and authors on how core chemical engineering subjects can potentially benefit from advanced educational digital tools. The opinions expressed by the respondents are shows as quotations in the table.

Table 2: Digitalisation of current practices and development of new competencies

Subject	**Digitalisation of current practices**	**New capabilities**

Thermodynamics	Visualization of Temperature composition diagrams can enable improved insights. Regression tools that can determine parameters for a given Equation of state (EOS) based on data.	Tools that can interactively calculate TXY information for a given EOS and parameters from a Vapor liquid equilibrium (VLE) library. As stated by a respondent “compare different thermodynamic package, understand the phase changes, and equilibrium processes.”
Mass and energy balances	Carry out basic mass and energy balance of a unit operation using digital tools. Visual aid to convey the basic concepts of mass and energy balances.	Tools that can enable multiple and complex scenario analysis. As discussed by a respondent “faster, tunable convergence, multiple simultaneous outputs from what-if scenarios, parameter changes that impact economics”
Heat and mass transfer	Analyze (and visualize) changes to heat and mass transfer as both the driving force and other parameters change.	Tools that enable the space dependent analysis of heat and mass transfer in all relevant situations. As discussed by a respondent “….,for complex geometries, spatially variable thermal properties and radiation”
Reaction and fermentation engineering	Numerically calculate the progression of a given reaction, Visualization of reaction progression and reaction types.	Scenario analysis enabling students to better understand how parameters and various reaction kinetics influence the overall fermentation process. As discussed by a respondent “keeping parameters under control for runaway prevention -

		linking tool outputs with real life consequences (simulator type)""
Separation processes	Numerically model separation processes, scenario analysis.	Model advanced separation processes with multiple components.
Process design	Scenario analysis, recycles and complex flowsheets. As pointed out by a respondent	Process optimization and integration combined with 3D and immersive environments.
Sustainability	Calculate impacts of carbon footprint	Integrated carbon footprint analysis from an early stage process design
Process dynamics and Control	Visualizations and implementation.	Real-time and hands-on analysis of controls enabled by OTS.
Safety	Visualization and scenario analysis	Connect decisions made in design to safety consequences and providing an immersive learning experience. As discussed by one of the respondents "Software with established complete systems/walk-around plant with scenario development and result analysis."

For many of the new capabilities listed above, the capabilities of process simulator, VR/AR and virtual labs/OTS platforms must be expanded. However, to do so requires developments and systems that can address the non-technical shortcomings of these core technologies.

The authors would also like to point out two current relevant trends that will inevitably change the landscape of digitalisation tools used in education. Firstly, there is a discussion within accreditation bodies, such as IChemE about the need for including cybersecurity into the curriculum, which has been identified as a gap in knowledge. Addressing this need effectively will require the use of digitalisation tools. Secondly, generative AI and large language models such as ChatGPT are becoming an increasingly available tool, and effective use these tools in chemical engineering education is inevitable. From a historical perspective these tools may require a similar change to the curriculum/teaching strategies that was warranted by the advent of process simulators.

Researchers/educators engaged in digital tool development will need to drive the digitalization of the chemical engineering curriculum. Be it with standard excel models or advanced virtual reality concepts. However, in order to make these tools more widely used in chemical engineering curriculum, chemical engineering educators who do not profess expertise must also be convinced to use these tools in their education. In reality, this means the barrier to switch over a course from their current delivery to a more digital tool centric delivery needs to be minimized. Part of the solution is developing training platforms and resources. For example text books that contains sufficient teaching and exercise material (Svrcek, Mahoney and Young, 2014) or other written resources that describe how a certain course can be taught (Udugama et al., 2020). In addition, at the university level educators/researchers engaged in digital tool development can conduct seminars to their colleagues which can be used for knowledge transfer. Alternatively, colleagues engaged in digital tool development can teach into a core chemical engineering subject, with the objective of familiarizing students with the use of digital tools in that given subject. Professional bodies that are pushing changes in digitalization, also needs to make resource available that can be used as reference work. At a faculty and university level, there is also a need to recognize that introducing digital tools into core engineering courses requires ordinary educators to pick up new skills, as such relevant extra time needs to be allocated. One model might be to treat an educator who has been teaching a core course and is attempting to introduce digital tools as an educator who is teaching the subject for the first time and updating course material, allowing them sufficient time and an incentive to update the course.

Conclusions

This manuscript set out to answer the question "how can digitalisation be used in chemical engineering education?". To facilitate this a survey was administered to a target audience consisting of Heads of Departments at IChemE accredited institutions and members of the IChemE committees focused on digitalisation. The 16 responses that were received were then analyzed and the following conclusions were made. Whilst the number of responses is relatively small, these responses represent a broad range of relevant expertise either from entire departments or from relevant technical committees. Mathematical/programming simplicity, ease of maintenance and low initial investment costs were identified as key non-technical aspects required for a prospective digitalisation tool. The respondents rated Microsoft Excel (VBA), commercial simulators and scripting tools such as Python and MATLAB as better platforms for a prospective digital tool than programming languages, CFD models, OTS, and VR/AR models considering the benefits to teaching and the non-technical hurdles that must be overcome to implement and maintain these tools. The respondents also identified that emerging technologies (in teaching) such as OTS and VR/AR have a role to play in areas such as process design and process safety. Considering these views, it is the authors' opinion that digitalisation of the chemical engineering education requires the use of a multitude of digital tools that can be based on Excel or scripting or a simulator, as well as on a VR platform. It is the authors' belief that widespread adoption of more advanced digitalisation tools will require the progressive dismantling of non-technical barriers to make them an interesting choice.

References

Alford, M., Udugama, I., Yu, W., & Young, B. (2022). Flexible digital twins from commercial off-the-shelf software solutions: a driver for energy efficiency and decarbonisation in process industries? Chemical Product and Process Modeling, 17(4), 395–407. https://doi.org/10.1515/cppm-2021-0045

A. Udugama, I., Munir, M. T., Kirkpatrick, R., Young, B. R., & Yu, W. (2018). Side draw control design for a high purity multi-component distillation column. ISA Transactions, 76, 167–177. https://doi.org/10.1016/j.isatra.2018.03.006

A. Udugama, I., Öner, M., Lopez, P. C., Beenfeldt, C., Bayer, C., Huusom, J. K., Gernaey, K. V., & Sin, G. (2021). Towards Digitalization in Bio-Manufacturing Operations: A Survey on Application of Big Data and Digital Twin Concepts in Denmark. Frontiers in Chemical Engineering, 3. https://doi.org/10.3389/fceng.2021.727152

Briones, L., & Escola, J. M. (2019). Application of the Microsoft Excel Solver tool in the solution of optimization problems of heat exchanger network systems. Education for Chemical Engineers, 26, 41–47. https://doi.org/10.1016/j.ece.2018.10.003

Calvo, L., & Prieto, C. (2016). The teaching of enhanced distillation processes using a commercial simulator and a project-based learning approach. Education for Chemical Engineers, 17, 65–74. https://doi.org/10.1016/j.ece.2016.07.004

Castier, M., & Amer, M. M. (2011). XSEOS: An evolving tool for teaching chemical engineering thermodynamics. Education for Chemical Engineers, 6(2), e62–e70. https://doi.org/10.1016/j.ece.2010.12.002

Chaves, G. L., Batista, R. S., de Sousa Cunha, J., Altmann, D. L., & da Silva, A. J. (2022). Teaching cellular metabolism using metabolic model simulations. Education for Chemical Engineers, 38, 97–109. https://doi.org/10.1016/j.ece.2021.12.001

Domingues, L., Rocha, I., Dourado, F., Alves, M., & Ferreira, E. C. (2010). Virtual laboratories in (bio)chemical engineering education. Education for Chemical Engineers, 5(2), e22–e27. https://doi.org/10.1016/j.ece.2010.02.001

Garcia Fracaro, S., Chan, P., Gallagher, T., Tehreem, Y., Toyoda, R., Bernaerts, K., Glassey, J., Pfeiffer, T., Slof, B., Wachsmuth, S., & Wilk, M. (2021). Towards design guidelines for virtual reality training for the chemical industry. Education for Chemical Engineers, 36, 12–23. https://doi.org/10.1016/j.ece.2021.01.014

Gargalo, C. L., Caño, S., Caccavale, F., Gernaey, K. V., & Krühne, U. (2022). Educational Computer-Aided Tools Towards Industry 4.0: Recommendations and BioVL (pp. 1273–1278). https://doi.org/10.1016/B978-0-323-85159-6.50212-8

Glassey, J., & Magalhães, F. D. (2020). Virtual labs – love them or hate them, they are likely to be used more in the future. Education for Chemical Engineers, 33, 76–77. https://doi.org/10.1016/j.ece.2020.07.005

Low, D. Y. S., Poh, P. E., & Tang, S. Y. (2022). Assessing the impact of augmented reality application on students' learning motivation in chemical engineering. Education for Chemical Engineers, 39, 31–43. https://doi.org/10.1016/j.ece.2022.02.004

Luyben, W. L. (2006). Distillation Design and Control Using AspenTM Simulation. John Wiley & Sons, Inc. https://doi.org/10.1002/0471785253

Martín, Á., Bermejo, M. D., Mato, F. A., & Cocero, M. J. (2011). Teaching advanced equations of state in applied thermodynamics courses using open source programs. Education for Chemical Engineers, 6(4), e114–e121. https://doi.org/10.1016/j.ece.2011.08.003

Norton, C., Cameron, I., Crosthwaite, C., Balliu, N., Tade, M., Shallcross, D., Hoadley, A., Barton, G., & Kavanagh, J. (2008). Development and deployment of an immersive learning environment for enhancing process systems engineering concepts. Education for Chemical Engineers, 3(2), e75–e83. https://doi.org/10.1016/j.ece.2008.04.001

Ramírez, J., Soto, D., López, S., Akroyd, J., Nurkowski, D., Botero, M. L., Bianco, N., Brownbridge, G., Kraft, M., & Molina, A. (2020). A virtual laboratory to support chemical reaction engineering courses using real-life problems and industrial software. Education for Chemical Engineers, 33, 36–44. https://doi.org/10.1016/j.ece.2020.07.002

Seifan, M., Robertson, N., & Berenjian, A. (2020). Use of virtual learning to increase key laboratory skills and essential non-cognitive characteristics. Education for Chemical Engineers, 33, 66–75. https://doi.org/10.1016/j.ece.2020.07.006

Selmer, A., Kraft, M., Moros, R., & Colton, C. K. (2007). Weblabs in Chemical Engineering Education. Education for Chemical Engineers, 2(1), 38–45. https://doi.org/10.1205/ece06018

Solmaz, S., Dominguez Alfaro, J. L., Santos, P., van Puyvelde, P., & van Gerven, T. (2021). A practical development of engineering simulation-assisted educational AR environments. Education for Chemical Engineers, 35, 81–93. https://doi.org/10.1016/j.ece.2021.01.007

Sunarso, J., Hashim, S. S., Yeo, J. Y. J., & Chew, J. J. (2020). MATLAB-based project assessment in process modelling unit: A case study from Swinburne University of Technology Sarawak Campus. Education for Chemical Engineers, 33, 17–26. https://doi.org/10.1016/j.ece.2020.07.001

Teles dos Santos, M., Vianna Jr., A. S., & le Roux, G. A. C. (2018). Programming skills in the industry 4.0: are chemical engineering students able to face new problems? Education for Chemical Engineers, 22, 69–76. https://doi.org/10.1016/j.ece.2018.01.002

Toyoda, R., Russo Abegão, F., Gill, S., & Glassey, J. (2021). Drivers of immersive virtual reality adoption intention: a multi-group analysis in chemical industry settings. Virtual Reality. https://doi.org/10.1007/s10055-021-00586-3

Udeozor, C., Toyoda, R., Russo Abegão, F., & Glassey, J. (2021). Perceptions of the use of virtual reality games for chemical engineering education and professional training. Higher Education Pedagogies, 6(1), 175–194. https://doi.org/10.1080/23752696.2021.1951615

Udugama, I. A., Bayer, C., Baroutian, S., Gernaey, K. V., Yu, W., & Young, B. R. (2022). Digitalisation in chemical engineering: Industrial needs, academic best practice, and curriculum limitations. Education for Chemical Engineers, 39, 94–107. https://doi.org/10.1016/j.ece.2022.03.003

Udugama, I. A., Gernaey, K. V., Taube, M. A., & Bayer, C. (2020). A novel use for an old problem: The Tennessee Eastman challenge process as an activating teaching tool. Education for Chemical Engineers, 30, 20–31. https://doi.org/10.1016/j.ece.2019.09.002

Viitaharju, P., Yliniemi, K., Nieminen, M., & Karttunen, A. J. (2021). Learning experiences from digital laboratory safety training. Education for Chemical Engineers, 34, 87–93. https://doi.org/10.1016/j.ece.2020.11.009

Wong, K. W. W., & Barford, J. P. (2010). Teaching Excel VBA as a problem solving tool for chemical engineering core courses. Education for Chemical Engineers, 5(4), e72–e77. https://doi.org/10.1016/j.ece.2010.07.002

Young, B. R., Mahoney, D. P., & Svrcek, W. Y. (2001). Real-time computer simulation workshops for the process control education of undergraduate chemical engineers. Computer Applications in Engineering Education, 9(1), 57–62. https://doi.org/10.1002/cae.1006

Yu, W., Patros, P., Young, B., Klinac, E., & Walmsley, T. G. (2022). Energy digital twin technology for industrial energy management: Classification, challenges and future. Renewable and Sustainable Energy Reviews, 161, 112407. https://doi.org/10.1016/j.rser.2022.112407

Zhang, Y., Munir, M. T., Yu, W., & Young, B. R. (2013). A real time approach to process control education with an open-ended simulation tool. Education for Chemical Engineers, 8(3), e105–e112. https://doi.org/10.1016/j.ece.2013.07.001

Highlights

- A survey was distributed to Heads of Departments at IChemE institutions and members of the IChemE committees focused on digitalisation.
- Identified key non-technical barriers to implementing digital tools in improving core chemical engineering education.
- Suggested use cases within in the core chemical engineering curriculum for currently available digitalisation tools.