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Teaching Computational Tools in Chemical Engineering Curriculum in Preparation for the Capstone Design Project

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ABSTRACT

UCL Chemical Engineering ensures graduates are digitally literate by integrating computational tools like gPROMS, Aspen Plus, and GAMS into the undergraduate curriculum. Students in the first year of undergraduate program use GAMS to solve simple simulation and optimization problems and gPROMS for solving ordinary differential equations (ODEs) in reactor design problems. In the second year, students start using Aspen Plus to simulate more complex chemical process units, interpret and discuss results obtained and justify any differences observed between experimental data and computational results. They use GAMS to simulate and optimize a process flowsheet with considerations of the implications of proper initialization procedures and strategies for obtaining optimal parameters and gPROMS for advanced reactor and separator problems. The computational knowledge acquired in the first two years prepares students for the third-year capstone design project where they use the various tools in designing and simulating their processes during the preliminary, conceptual and detail designs. The computational resources available to students and the additional supports provided by educators help the students succeed on the design project in the third year. This work outlines strategies for delivering the computational tools required for modules in the first two years of the undergraduate program and the application of the knowledge in the third-year design project. It demonstrates how complex process systems engineering (PSE) problems are taught, student support and resources available, and feedback for continuous improvement. It presents some challenges faced due to the use of generative AI tools and how this can be addressed.

Keywords: Education, Aspen Plus, GAMS, gPROMS, Process Design, GenAI

INTRODUCTION

Computational tools are present in most, if not all, Chemical Engineering programmes according to Molaei Chalchooghi and Sorensen [2]. In the digital era we live in, universities prioritise that their graduates are digitally literate, able to use a variety of digital tools. These computational tools could range from process simulators, programming languages, computer packages etc., and are widely used both in academia and industry for solving several problems, from the solution of very simple algebraic equations to the optimisation of complex (i.e. highly non-linear and non-convex) processes and flowsheets [3]These tools include, but are not limited to, Aspen Plus [4], GAMS [5], gPROMS [6], ChemCAD [7], MATLAB [8], Python [9] etc. Some of these tools, among others, are widely used in Chemical Engineering programmes, due to their ease of use, accessibility, availability of teaching and learning materials and resources [10], however, the choice of tools to be used depends on the application, the level of the students etc.

Computational tools in chemical engineering are essential for process design, simulation and optimization and for solving complex problems [11]. Tools like Aspen Plus can be used to model chemical processes, simulate plant operations, and optimize process conditions. These simulators allow engineers to design and test process configurations before physical implementation, reducing cost and risk. While gPROMS ModelBuilder can be used for dynamic simulation and optimization, parameter estimation, experimental design etc, General Algebraic Modelling System (GAMS) is designed to solve large scale optimization problems. Within the Chemical engineering program, it can be used for process optimization, production planning and scheduling, heat integration and energy management through heat exchanger networks optimization, process synthesis and economic evaluation of processes.

This work explores the approach to teaching computational tools in the first two years of undergraduate chemical engineering program at UCL. It discusses the design of teaching methods, assessment strategies and feedback, along with the development of learning resources and the challenges encountered. Additionally, it highlights the collaborative efforts between students and staff in enhancing computational education and addressing learning difficulties, ensuring students are well-prepared for the third-year capstone design project and beyond.

COMPUTATIONAL TOOLS TEACHING, ASSESSMENT AND FEEDBACK APPROACHES

Teaching Approaches and resources

In the department, students are taught how to select the most suitable software for a given problem; and how to use this software effectively in their work before proceeding to solve more challenging problems in their future careers. In addition, teaching staff regularly evaluate the material delivered, to ensure that the concepts and topics discussed align with current research directions and the constantly evolving industrial needs.

The teaching approach includes a combination of lectures, video tutorials, and guided problem-solving sessions, ensuring students have multiple avenues for learning and understanding these tools. Supporting resources such as tutorial videos and lecture slides have been developed to cater to diverse learning needs and allow for self-paced learning.

In the first year of the undergraduate program, students are introduced to GAMS (General Algebraic Modeling System) and gPROMS Model Builder as part of the Computational Modelling and Analysis module. These tools are fundamental in developing computational problem-solving skills relevant for the chemical engineering degree program early in the curriculum. For GAMS, they learn how to solve various problems, starting from basic systems of equations to more applied cases such as simple flash calculations and refinery blending problems. The problems are carefully designed to expose students to different solvers, including constrained non-linear systems (CNS), linear programming (LP), and non-linear programming (NLP) solvers. By working through these exercises, students gain a good foundation in optimization and numerical methods, while developing a good understanding of how different mathematical formulations are applied to practical engineering problems.

For gPROMS, students are taught how to solve basic ordinary differential equations (ODEs) before progressing to more complex problems involving batch and continuous stirred tank reactors (CSTRs). This provides them with an understanding of dynamic systems and the ability to simulate basic reactor problems.

In the second year, students build on their foundational knowledge by tackling more advanced problems using GAMS. They are tasked with solving process design challenges involving complex flowsheets that typically include a flash column, a reactor, heat exchangers, and separation units. The entire process flowsheet is implemented in GAMS, requiring students to integrate multiple unit operations into a cohesive optimization framework. This includes defining an objective function, such as maximizing product yield as well as economic potential or minimizing energy consumption with the use of relevant optimization solvers. Through these activities, students further develop their programming and modeling skills and become more aware of process design and optimization concepts that are relevant to real-world engineering practice.

Additionally, Year 2 introduces students to Aspen Plus in the Separation Processes module in three lectures, integrated within the module curriculum. During these lectures the students are introduced to the Aspen plus as a simulation tool and its application in chemical engineering. They begin by learning to model basic processes, such as heaters, coolers, short cut distillation models (DSTWU), and liquid-liquid extraction. These foundational exercises build their confidence to tackle more complex operations, including rigorous distillation with RadFrac. As the course progresses, students explore advanced tools within Aspen Plus, such as sensitivity analysis for optimization and economic feasibility studies to assess the viability of process designs.

The teaching approach and computational topics covered during the year 1 ,2 and 3 are summarised in Figure 1. This approach ensures that students are equipped with the skills needed to select the most suitable computational tools for specific problems and reflect on their results before their third year capstone design project.

During their studies, students have continuous access to online learning material for all the computational tools used across the entire curriculum (i.e. AspenPlus, gPROMS, GAMS and MATLAB). The material for each of the tools includes how-to videos and step-by-step presentations that explain various concepts and processes, and how these can be implemented and solved using the respective tool. The material is updated regularly to make sure it aligns with the theory taught, or any new elements added, as well as updated versions of the software. For instance, material on how to consider distributed models in gPROMS, and relevant examples thereof, is available for students to download, study and apply in their own time. Relevant material is available online also for aspects that are not formally considered or assessed as part of any of the taught modules, such as solids processing, so that students can refer to this if they need to consider these aspects as part of an open-ended project. Postgraduate students also make use of these resources as needed in their research and taught modules.

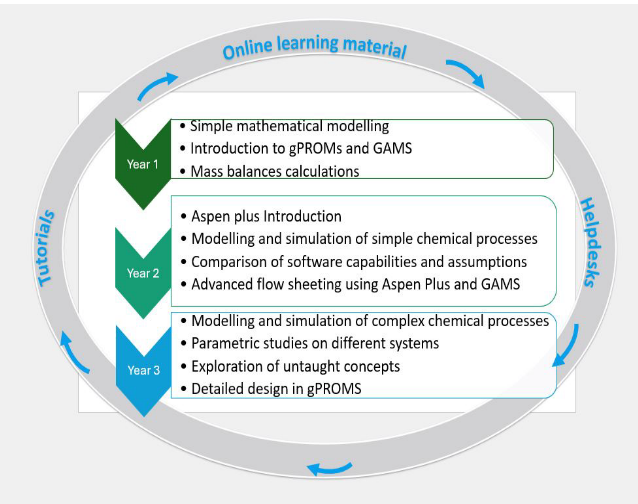

Figure 1. Distribution of PSE related tasks and available support over the curriculum.

This supporting material provides additional resources that are useful to the students especially for their projects in 3rd year, when they need to consider processes not previously covered in individual taught modules [1].

ASSESSMENT APPROACHES

Assessments Approaches

In all modules discussed in the previous section, assessed projects and team reports evaluate whether the learning outcomes are met, whilst tutorials for the relevant computational tools take place before the release of the material for which the software is required (e.g. project, coursework etc.). In addition, computational help desk sessions are scheduled before the respective assessment deadline so that support by staff is provided to students who may be facing difficulties with the specific software used.

In Year 1, in Process Modelling and Analysis module, students apply their computational knowledge through assessments that account for 50% of the overall module grade. These assessments include both coursework and project designed to evaluate their knowledge of using GAMS and gPROMS for programming and modelling. The problems presented to students cover a wide range of applications, including but not limited to application of some numerical methods, process flowsheeting with recycles, sensitivity analysis, convergence analysis, and simulation of steady-state and dynamic operations by solving relevant ordinary differential equations (ODEs).

In Year 2, as part of the Process Design Principles module, students undertake a project that constitutes 60% of the overall module grade. In this project, students use GAMS and Aspen Plus to design a complete process plant. The project involves solving a complex problem with multiple design variables, where the primary objective is typically to maximize the economic potential of the process and obtain a stream table for the process. Students are required to compare results obtained in GAMS with that of ASPEN and comment on the discrepancy observed. Within this assessment, students perform sensitivity analyses to identify the optimal set of operating parameters that achieve the best economic potential. This task requires the application of advanced features in GAMS, such as the use of flow-control structures (e.g., while loops), enabling them to handle iterative calculations effectively. The project provides students with hands-on experience in tackling design problems and reinforces their understanding of process design, optimization, and modelling using computational tools. Refer to **Table 1** for Computational tool used in year 1 and year 2 as part of different modules' assessments. These assessments are designed to not only test students' technical understanding of the computational tools but also to develop their problem-solving skills and confidence in applying these tools to real-world chemical engineering challenges.

Artificial Intelligence (AI) Tools and Assessment

Technological advancement has introduced unique challenges in assessment involving the use of computational tools, particularly with the increasing accessibility of AI tools that can generate code in common programming languages such as Python and MATLAB with high accuracy. One of the primary challenges is the potential misuse of these AI tools by students to generate code required as part of their assessment. While these tools could be valuable aids, their misuse can diminish students' critical thinking and proficiency in using the tools. For instance, rather than developing a good understanding of model implementation in these software, students might rely solely on AI-generated solutions.

The situation is further aggravated by the flexibility offered to students in some assessments, where they are free to choose the software or tools they prefer. In these instances, the use of AI assistance could undermine the intended learning outcomes if assessments are not carefully designed.

Table 1: Computational tools used in different modules in Year 1 and 2.

Year of study	Module name	Computational tools used
Year 1	Process Modelling and Analysis,	GAMS and gPROMS Model Builder
	Design and Professional skills I	GAMS
Year 2	Separation Processes	ASPEN PLUS and gPROMS Model Builder
	Process Design Principles	ASPEN PLUS and GAMS
	Design and Professional Skills II	ASPEN PLUS and GAMS

To address this, educators need to adopt strategies that ensure assessments meet their educational goals even when students have access to AI tools. Assignments should be structured in a manner that integrates critical analysis, interpretation of results, and the ability to explain the rationale behind specific computational approaches. For example, tasks that require students to debug, modify, or evaluate AI-generated code can shift the focus back to understanding the implementation rather than just copying the generated codes. Similarly, incorporating reflective components, where students justify their approach to solving a problem, can help educators gauge their understanding.

UCL has also provided a guideline on how generative AI (GenAI) can be used ethically in assessments. Students must acknowledge where and how they have used GenAI in any piece of work they are submitting, and where GenAI is used inappropriately, this is considered academic misconduct that will be referred to the appropriate panels.

FEED BACK APPROACHES

The application of computational tools is integrated within the curriculum of different modules as presented in **Table 1**. Students' feedback is collected formally three times per modules as part of CMD (continuous module dialogue). UCL's approach to gathering and responding to student feedback prioritizes anonymity and open communication, ensuring students felt comfortable sharing their experiences and suggestions.

To collect feedback effectively, Mentimeter slides are used, which allow students to present their feedback anonymously. This method was chosen to encourage honest communication, ensuring that students could express their views without hesitation [12]. By using this approach, a wide range of perspectives on the students' learning experiences are gathered, along with the challenges they faced, and their suggestions for improvement. After collecting feedback on learning experiences and challenges, the module coordinator analyses the responses and the proposed actions for developing the delivery of computational tools were collaboratively discussed with the teaching team. To maintain transparency, response slides are uploaded to Moodle, ensuring all students have access to the comprehensive overview of the improvements made based on their feedback.
Student feedback over four years for the *Computational Modelling and Analysis* module (Year 1) showed positive responses, with low response rates of 29%, 26%, 27%, and 41%. 75% found the materials useful, and 66% said tutorials met expectations. Feedback led to improvements, enhancing student confidence. Future efforts will address challenges to improve learning outcomes further.

APPLYING COMPUTIONAL TOOLS IN THE CAPSTONE DESIGN PROJECT

During the Capstone Design Project, students apply the knowledge of computational tools they have developed over their first two years of study to design and optimize a chemical plant. The project is structured into four main stages: Appraise, Select, Unit Design I, and Unit Design II. Computational tools are used in the first three stages the details of which are provided in this section.

In the Appraise stage, students begin by developing a mathematical model of the process plant. Using GAMS, they solve the mass and energy balances for the entire process. This enables them to produce a comprehensive stream table for the flowsheet and estimate the energy requirements for the plant.

In the Select stage, students create a detailed Process Flow Diagram (PFD) and simulate the entire process in Aspen Plus. This simulation helps them assess the initial feasibility of the process and apply heat integration principles to optimize energy recovery for the overall plant, improving efficiency and sustainability.

Finally, during the Unit Design I (UDI) stage, students focus on the detailed design of a major process unit, such as a reactor or a separator. For separation columns, they use Aspen Plus, leveraging its robust capabilities in simulating and designing such systems. For reactor design, students are given the flexibility to choose from various computational tools as they wish. Commonly chosen tools include gPROMS, Python, MATLAB, and Polymath, each offering distinct capabilities for modelling and optimization of chemical processes. For more information on the design project stages, refer to Nayak-Luke et al. [13]

TEACHING APPROACHES OF COMPUTATIONAL TOOLS IN THE DESIGN PROJECT

In the context of the Capstone Design Project, our teaching approach includes providing structured technical support sessions to assist students in overcoming computational challenges. These sessions are designed to address the diverse technical difficulties faced by students, ensuring that they can effectively simulate and analyze their chemical engineering processes using computational tools.

To facilitate effective learning, the technical support sessions are conducted in small groups of 10-15 students. This group size allows for personalized attention, fostering student engagement and encouraging active participation. Each session is repeated four times depending on the size of the cohort to accommodate different groups of students, ensuring consistent delivery of content across all sessions. The structure of these sessions is informed by educational frameworks [14] and aligned with the key aspects of teaching.

In preparation for each session, we create a forum where students could submit their questions in advance. This approach enabled the teaching team to identify the key issues to be addressed during the session, optimizing the use of time and ensuring that the most pressing concerns were covered. Additionally, this forum allows students who might be hesitant to ask questions during the session to voice their concerns anonymously, fostering a more inclusive learning environment.

The main challenges encountered during these sessions included maintaining consistent content delivery across different groups and addressing all student questions within the limited time available. Moreover, managing the varying levels of simulation skills among students required careful formulation of responses to ensure that all students could understand and apply the information, regardless of their progress.

While the primary focus of the sessions is to provide computational support, an equally important objective is to bridge the gap between theoretical knowledge and practical application. By interpreting the results generated by the computational tools, students are encouraged to critically evaluate whether the outcomes were reasonable in the context of the theoretical concepts they had learned in previous years. This integration of theory and practice is crucial for developing a deep understanding of chemical engineering principles.

Following each session, a comprehensive Frequently Asked Questions (FAQs) document addressing the main points discussed is uploaded. This resource is made available to all students, including those who are unable to attend the sessions or those that had fewer questions asked during their session. The FAQs document serves as a reference, allowing students to revisit key concepts and solutions as they progress through their design projects

STUDENT-STAFF COLLABORATIONS IN DEVELOPING THE RESOURCES FOR COMPUTATIONAL TOOLS

UCL is committed to fostering staff-student collaboration through projects aimed at enhancing the quality of teaching and learning across departments. The need for student-staff partnership in teaching and learning and its benefit has been documented in literature [15]. In summer 2024, the Faculty of Engineering Sciences funded a project in the Department of Chemical Engineering at UCL to address specific areas where students expressed a need for additional support in computational tools. One such project involved a student developing computational resources over two months, focusing on topics that posed challenges for their peers. These resources included: step-by-step guides (in PowerPoint and Word format) on retrieving experimental data from Aspen, instructions on implementation of column internals for distillation columns, detailed troubleshooting workflows for resolving issues in AspenPlus for increasingly complex chemical processes, and guidelines for configuring more advanced process intensifications in AspenPlus, specifically reactive distillation columns. These materials were made available students on the department's online learning system (Moodle) to provide accessible and structured support for students across all cohorts. They are designed to assist students with coursework and project and to enhance understanding of advanced process simulation topics. Additionally, a similar summer project was undertaken by another student to develop resources aimed at simplifying basic modeling concepts and learning videos and slides on GAMS and gPROMS. The developed materials from this project included: sample GAMS and gPROMS codes for fundamental modeling tasks, troubleshooting tips for common errors in GAMS, and a collection of exercise problems tailored to engineering applications. These materials have also been made available to students on the online learning platform.

The active involvement of students in developing these resources not only addresses immediate learning gaps but also promotes continuous improvement in the teaching of computational tools. This collaboration highlights the value of leveraging student perspectives to improve learning resources and accessibility, while simultaneously equipping them with practical skills in computational problem-solving that could be developed further in the future.

CONCLUSION

This paper outlined the integration of computational tools within the undergraduate chemical engineering curriculum at UCL, specifically in preparation for the third-year Capstone Design Project. It presents the approach to teaching these tools, the assessments, the feedback received from students and how it is responded to, and the various support mechanism provided to facilitate their learning.

Students are introduced to computational tools in their first year, where they apply them to solving fundamental chemical engineering problems in process modeling and simulation which they further develop in their second year by tackling more complex problems involving process design and optimization. This prepares them for them for the capstone design project in the third year.

The rapid advancement of artificial intelligence presents new challenges in higher education, particularly regarding academic integrity and the potential over-reliance of students on AI-generated solutions. Addressing these concerns requires the careful design of assessments that emphasize critical thinking and problem-solving, ensuring that students develop the deep understanding necessary for professional practice.

By continuously refining the integration of computational tools and adapting teaching strategies to evolving technological trends, chemical engineering education can better equip students with the skills needed for both research and industrial applications.

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