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# Recent Evolutions and Trends in the Use of Computer Aided Chemical Engineering for Educational Purposes at the University of Liège

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## Abstract

The present paper addresses the evolution and perspectives in the teaching of CAPE methods in the Department of Chemical Engineering at the University of Liège. The transition that happened in the 90ies with the arrival of commercial software is highlighted, as the learning outcomes evolved from the ability of building programs to solve chemical engineering problems towards the ability to use complex commercial software and to understand their limitations. Moreover, CAPE methods were extended to non-dedicated CAPE courses, which is illustrated here by the goals and challenges of their use in courses like “Reactor Engineering” and “Life Cycle Analysis”. It was observed that students sometimes assume that CAPE softwares provide straightforward and trustworthy solutions without the need of understanding their mathematical bases and assumptions. Thus, solutions to make students aware of these limitations are proposed, including the creation of an integrated project focussing on complex multi-disciplinary issues, evidencing the need for critical input from the operator.

**Keywords**: CAPE teaching, Education evolution, Integrated project, Reactor engineering, LCA.

## 1. Introduction

The discipline known as Computer Aided Process Engineering has seen a fast evolution since its birth in the sixties, and the education methods to train students have evolved accordingly. With increased complexity and capabilities of CAPE tools, new challenges have appeared and the teaching scope has evolved. Originally focussing on the ability to develop, program and use computational models for solving chemical engineering problems, it has shifted towards the ability to understand and use commercial black box software with user-friendly interface (a typical example is Aspen Plus). Moreover, the use of CAPE tools in education has been extended to many courses of the chemical engineering curriculum. Teaching challenges include the training of students to address not only isolated analytical problems but also multi-layers complex systems integrating many disciplines. In this sense, CAPE tools are a unique opportunity for students to manage the complexity of large integrated problems in a global approach (Pintarič and Kravanja, 2016). The present paper studies the past and present educational challenges related to CAPE tools, with a focus on solutions implemented at the University of Liège both at the Bachelor and Master levels. Then, the challenge of integrating the different courses within a common project using CAPE tools is discussed.

## 2. Retrospective and recent developments in CAPE teaching at ULg

In the present paper, the attention is set on the first (bachelor) and second (master) cycles of the chemical engineering education as established by the Bologna reform.

### *2.1. First contacts with programming and CAPE tools in the 1st cycle*

At the University of Liège, all engineering students follow a common educational pathway during 3 semesters before choosing any optional courses. In the common courses, students have an introduction to the Basics of Informatics and Algorithmics. The learning outcome principally consists in being able to analyse and solve middle-size problems by creating efficient algorithms. A second traditional course at the Bachelor level is Numerical Analysis, teaching students numerical methods for equation solving as well as the basics of linear programming. In addition to the practical exercises included in these courses, students follow a Project Course to gain practical experience in programming and use of numerical methods. In this course, groups of 3 students use Matlab to solve a general engineering problem. Besides the curriculum common to all engineering students, students orienting themselves towards chemical engineering also follow an Introduction to Chemical Engineering and Industrial Processes. This course has been recently introduced with the objective of briefly sketching the main challenges of process engineering to undergraduate students. It focusses on writing mass balances for different kinds of equipment and processes with or without reactions. The goal is to make students aware of the universality of mass balances, and to teach them a 4-step solving methodology consisting in (i) analysing the problem, i.e. translating the statement into a process scheme with identified variables, (ii) determining the number of degrees of freedom, (iii) writing the equations (mass balance, specifications…) and solving them in Matlab or any equation solver, and (iv) checking the validity of the solutions. The learning outcome is that students identify the methods and principles of closing balances in Process Engineering. This course also teaches students to recognize and use specific terms such as recycle, purge, yield, selectivity…

### *2.2. Dedicated CAPE research and teaching in the 2nd cycle*

The University of Liège (ULg) has a long tradition of using and developing CAPE tools dating to the seventies, when former Professor Boris Kalitventzeff created the LASSC (Laboratoire d'Analyse et de Synthèse des Systèmes Chimiques), joining what is now the Department of Chemical Engineering. In 1972, the first programmable calculator for the Department was purchased (Wang calculator) and connected to multiple monitors to be available for 3 persons at a time. First research projects using CAPE at ULg focussed on solving typical industrial process flowsheets such as ammonia or methanol synthesis (Kalitventzeff et al., 1973). Later in the 70ies, first personal computers appeared, and research projects extended to thermodynamics, with the development of databanks and equations of state (e.g. Heyen, 1980). From 1978, the rational use of energy in industrial processes became an important topic in the LASSC whose activity focussed on the development of validation tools, resulting in the creation of the Belsim software, now commercialized under the name Vali by the company Belsim SA. In the 1990ies, numerous works on energy integration in the industry were realized (e.g., Maréchal et al, 1998) and from the turn of the century, different topics were studied like detailed boiler models (Dumont and Heyen, 2004) and dynamic validation (Ullrich et al., 2010). More recently, environmental issues gained in importance with research in data mining for emission control (Sainlez and Heyen, 2012) and $CO_2$ capture (Léonard et al., 2015). These last topics are still among the interests of CAPE research at ULg.

From very early on, CAPE experience gained in research projects was used to illustrate dedicated courses. Along with first master's theses, the teaching of CAPE methods started as early as 1972 with the courses of "Simulation and Optimization of Chemical Systems" and "Dynamics and Command of Chemical Systems". The teaching partly focussed on training students to generate FORTRAN code sequences to solve chemical engineering problems, like e.g. liquid-vapour equilibrium or plug-flow reactor discretization. With time, more and more routines were provided to students who could also benefit from an easier access to hardware and to thermodynamic databanks. In the 90ies, the appearance of commercial softwares initiated a shift in the teaching objectives as the goal became slowly to train students to identify the potential and limitations of modelling. The use of commercial software allowed for increased complexity of the models built by students. However, the need for programming decreased, and it ended up disappearing from dedicated CAPE classes at the Master level. As an identified consequence, it was observed that students were losing some understanding of the physical and mathematical bases that support process simulation software. This sometimes led students to skip the "conceptual model step", i.e. to directly create models in the user-friendly black box software before getting enough awareness about the problem set. In other words, they sometimes use process engineering software as "drawing tools" that provide straightforward and presumably reliable answers rather than as complex equations solvers that require critical operator input. As such software provides many initial guesses (e.g. heat exchange transfer coefficient, units for kinetic constants…), students consider these guesses as trustworthy standard values, and they neglect to check the available descriptions of the numerical models assumptions.

Two main solutions have been implemented to address these issues. The first one consists in drawing the student's attention on these issues during the theoretical and practical CAPE-dedicated classes. For instance, the general principles of modelling (not only applicable to chemical engineering) are given a special attention in the theoretical classes, insisting on the comprehension of the real problem and the elaboration of a conceptual model before its implementation. In addition, mathematical models for process blocks and solving methods are not only discussed in the theoretical classes, but also in the practical classes, in relation with the use of commercial process simulation software. Students are thus asked to study the hypotheses and mathematical models used in the software. For instance, they have to identify variables and equations for typical physical unit operations, and to relate the resulting number of degrees of freedom to the number of specifications required in the black box model implemented in the simulation software. The acquisition of these skills is an important part of the final grade, made up from both practical classes' reports and examination. Then, the second solution is related to the introduction of an integrated project that counts for 10 credits (over 60) in the first year of the chemical engineering master. Expected CAPE learning outcomes and challenges of this project are described in section 3.

### *2.3. Non-dedicated CAPE research and teaching in the 2$^{nd}$ cycle*

With time, the use of CAPE has broadened and computers now contribute to solve common problems in all process engineering disciplines. Associated teaching is illustrated with two examples: "Life cycle analysis" and "Reactor engineering" courses.

#### *2.3.1. Use of CAPE tools in the course of Life cycle analysis*

Life Cycle Assessment is taught to chemical engineering students during their last year of studies. The course is divided in three parts: (i) learning, (ii) practicing, and (iii) acting with an open mind. The first part highlights the main environment challenges for current and future generations. Students also learn the specific LCA methodology described in ISO standards using mainly exercises and examples from the literature. As the second part is dedicated to practice, students also learn to use LCA software. They practice by modelling and implementing scenarios (same for all students) in the software. Due to the large amount of data needed for an LCA, a software tool is very useful to reduce the complexity and the time to assess the environmental impact of a process or a product. Students also have to perform energy and mass balances without software. Indeed, the main drawback is that students may not analyse the sense of the simulation results. They sometimes just "push the button", get results and believe them. As a consequence, teachers pay a special attention to illustrate with examples that the simulation software is only a tool (or an interface) and that data quality is of paramount importance. Results obtained by students must thus be explained and justified using their critical thinking. The most important learning outcome for students is to analyse results and to understand the limitations of the tool and when its use is not relevant.

In the third part of this course, students in groups receive a scientific paper, different for each group and describing topics ranging from insulation and building design to food logistics. The groups have to criticize the paper, showing its environmental relevance and its (non-) accordance with the ISO standards. They model the scenarios using available data and software. The goal is to understand the difficulty of the modelling, the importance of choices relative to databases and how to deal with software results. Students also compare their results with the published ones and need to justify their results and the possible discrepancies. Teachers do not evaluate the modelling results but the approach used by the groups and how students interpret the results. Indeed, as for every CAPE tool, it should be highlighted that LCA software should not be used as a black box without understanding the process or the product modelled. The conclusion sentence of the lecture summarizes the sense of what teachers would like students to learn from this lecture: "Be careful. This machine has no brain. Use your own".

*2.3.2. Use of CAPE tools in the course of Reactor Engineering.*

In this course, the students apply theoretical concepts through the modelling and simulation of a chemical reactor. In order to get a good understanding of the mathematical methods, they write themselves the equations (mass and heat balance) describing the reactor behaviour and do not use pre-built models. This implies that students have to select the reactor model (batch/continuous – plug flow/perfectly mixed) in relation to the design and operating mode of the industrial reactor to be simulated. Equations are solved numerically using tools such as Matlab or Polymath. As no parameter values are provided by the software, students collect data by themselves: kinetic equations, reaction enthalpy, thermodynamic data… They thus have to develop critical thinking in the choice of the equations and the building of the conceptual model.

The use of numerical tools to integrate balance equations also allows students to make numerical experiments. They may test, simultaneously or not, broad ranges of operating conditions and parameters values. These sensitivity analyses allow them to better identify the most influencing parameters, the necessity (or not) to get more accurate values for selected variables and parameters. The learning outcome is to make students more aware of the physical meaning of all terms and parameters which have to be considered to simulate a reactor. Such a project thus intends to fill the gap between the very simple problems which may be solved "by hand" (usually used to illustrate the reactor modelling theory), and the pre-built reactor models proposed in CAPE software.

## 3. Integrated project as a case study for the teaching of CAPE

Although CAPE teaching has been broadened to several courses, a global approach was still missing, and the relevance of CAPE tools for managing the complexity of current chemical engineering issues needed to be better highlighted. Simultaneously, looking at general trends in the chemical engineering teaching, the integration of multiple technical and soft skills into a common project was recommended by University authorities and industrial partners as well as by international experts (AEQES, CTI) that evaluated the education quality of the Chemical Engineering master at ULg. Among other improvements, an integrated project focusing on energy-transition issues was created to replace the former "Plant design project". This new project was built as an innovative teaching method for students in teams of 5 to 10 members to acquire the technical and soft skills needed to address multi-disciplinary topics. Indeed, it was observed that students usually treated each course separately rather than considering the education as a whole. Besides the required work in large teams, one of the main challenges of this project course is thus to encourage students to understand chemical engineering as a global and multi-faceted topic, with many related sub-disciplines.

The integrated project is structured in 3 parts taking place over two semesters. First, students analyse a large and complex energy system, typically a well-delimited region: Reunion Island or the Walloon region have been recently proposed. In their analysis, students propose a reasonable energy map at the region scale following a few constraints imposed by the teachers and related to energy-transition issues like the use of a sustainable chemical energy carrier or the replacement of a relevant percentage of fossil natural gas by bio-methane. As the studied system is selected to be large and with many unknown variables, its complexity and its behaviour can only be assessed by the use of tools such as Excel models and Sankey diagrams. In the second part of the project, students follow the hierarchical approach to design the (bio)chemical process(es) that allow the transition towards this more sustainable energy map. They study each physical unit operation separately and size them according to their initial energy map, using equations solving software like Matlab. They also implement physical unit operations separately in process analysis software such as Aspen Plus. Finally, in the third part, students implement the whole process model into Aspen Plus and they use it to evaluate the performances of the integrated process.

In this context, CAPE tools play an important role as they help students to get a global overview of the process supply chain (part I), to design and size the equipment (part II), and also to integrate the different blocks and study the global flowsheet (part III). Moreover, the open problem statement forces students to design and size process (almost) from scratch and thus to create the conceptual models to be implemented in the second and third parts. As a result, they get a feeling about what parameters are important for each physical unit operation (flow rates, purities, energy demand…). They also need to pay attention to the hypotheses made by commercial softwares to make sure that the implemented models respect the specifications of their conceptual models.

The learning outcomes are that students analyse large multi-disciplinary problems, work efficiently in large teams (support is provided by the Psychology Department), and design (bio)chemical processes. Regarding CAPE, the main outcome is that students use CAPE software with critical mind to reach the large and complex objectives of the initial problem assignment. Students are evaluated on the final solution to the complex problem but also on their ability to communicate these results orally (presentations at the end of each project part) and in writing (reports in parallel with the oral presentations). Their behaviour within the team is assessed by peers and it individually influences the student's grade, starting from the overall grade obtained by the group. Qualitatively speaking, it was observed that this project helped most students to gain in maturity: they appeared to be more aware of orders of magnitude, verified the obtained results before presenting them to the class, and they learned to make relevant assumptions to solve the problems faced. However, it also appeared that the project results were strongly depending on the team organization, the full support of all team members being necessary for the project to be successful.

## 4. Conclusions

The importance of educating students to critical thinking when using CAPE tools has been evidenced in dedicated CAPE courses, as well as in courses where the use of CAPE methods is more recent. A retrospective on CAPE teaching history at the University of Liège has evidenced that the challenges, the objectives and the scope of the education to CAPE methods have significantly evolved. Among other proposed solutions, the integrated project developed at the University of Liège make students aware of the CAPE tools potential to analyse and solve large and complex problems, and it forces them to understand and select appropriate mathematical methods and process assumptions when using commercial softwares (Matlab, Aspen Plus, Belsim Vali…). Besides the ability to work in large groups, this project thus also requires students to develop critical thinking to succeed in their work as chemical engineers.

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