

BOARD # 46: Work-in-progress: Evidence-based scope and selection of threshold concepts for the design of computational notebooks in undergraduate statistics courses for chemical engineering

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Abstract

Computational tools continue to gain popularity across engineering curricula. Computational notebooks, such as Jupyter, Google Colab, and MATLAB live scripts, allow dynamic interactions between instructors and students with immediate feedback on a given topic. However, there are limited guidelines on how to design these computational notebooks to intentionally enhance student learning, specifically what concepts to include in the notebooks. There is limited literature on this topic in the context of general engineering education, especially at the undergraduate level. In this work-in-progress, we focus explicitly on an undergraduate introductory statistics course for students in a chemical engineering program. Our overarching research goal is to devise how these computational notebooks indeed facilitate student learning in the context of undergraduate instruction. We first engage in identifying relevant statistics concepts for chemical engineering that could be identified as threshold concepts (TCs). These are concepts that are essential for building understanding and applying the rest of the content in a course or subject. Therefore, the goal of this paper is to conduct a literature review of TCs related to undergraduate statistics for chemical engineering. We start with the current knowledge on the TCs in general undergraduate engineering education, present the common approaches for mapping and assessing TCs in engineering courses, and discuss specific works related to statistics courses for undergraduate students to showcase the main roadblocks students face when learning statistics and data analysis. This literature review will serve as a baseline to establish a set of concepts that will offer critical learning areas to focus the design of computational notebooks in the context of undergraduate chemical engineering education.

Keywords: computational notebooks; threshold concepts; undergraduate education; cognitive apprenticeship model; STEM computational tools

Introduction

How students learn and how to facilitate this process are long-standing questions in education in general. Efforts to develop formal pedagogical frameworks to identify specific roadblocks and address them are prevalent in engineering education research. Some strategies that have shown increased performance in engineering students include cooperative learning, active learning classrooms, flipped-courses, and interactive assignments [1]. Some of these strategies are easier to implement in the context of engineering courses, while others require more intentional design to accomplish the desired learning outcomes of a given course.

Chemical engineering students are trained in different approaches to solve complex mathematics to model fluid dynamics, heat and mass transfer, kinetics, process control, and data analysis. In some courses, numerical methods and basic programming skills are also introduced at the undergraduate level. Specifically at our institution, which is a large public state university in the Northeast United States, chemical engineering students complete a series of four laboratory courses, each associated and taken concurrently with specific core chemical engineering courses

in the junior and senior years. The first of these lab courses intends to prepare students for appropriate use of graphs to represent data, evaluate uncertainty, and use basic statistical analyses to provide objective assessment of a process. This lab is usually taken in tandem with the *Probability, Statistics, and Data Analysis* course, which is taught in the department. Anecdotally, the concepts that students struggle with the most in this chemical engineering statistics course are (1) differentiating sample from population and (2) defining a random variable and determining how to properly define it in a problem. These concepts are key to understanding and applying the rest of concepts covered in the statistics course; as such, these are threshold concepts (TCs).

Some disciplines use TCs or *core concepts*, interchangeably, but this is not true in all fields. There are more studies on TCs and their implementation related to social studies, business, and health sciences [2-6], with fewer research publications in the context of general engineering education. Furthermore, current practice to identify TCs in engineering courses largely relies on instructor experience over multiple terms teaching a given subject and student surveys [7-10]. TCs are "gateways of knowledge" that transform the student's understanding of a topic and a discipline. As such, there is urgent need to develop evidence-based protocols to identify TCs and drive conversations about effective teaching. Understanding how students learn and the roadblocks that impede their learning will enable improved course design, assessment of learning outcomes, and instructor training and development [11-13].

This work-in-progress is the first step in a two-year study to determine scaffolding techniques that will enrich the learning experience of undergraduate students in chemical engineering with respect to selected TCs in undergraduate statistics. The long-term goal of the project is to formally investigate factors that contribute to student engagement, learning, and performance in undergraduate engineering courses. Few studies address evidence-based design of computational notebooks for engineering courses [14, 15]. In this project, we explore computational notebooks as a scaffolding tool to help students develop a skillset they can translate to different working environments beyond their undergraduate education. Our curricular innovation intends to systematically design and assess computational notebooks to facilitate learning of selected TCs, starting from the premise that research-based design of computational notebooks can significantly facilitate student learning. This literature review is intended as a baseline to establish a set of TCs that will offer critical learning areas to focus the design of computational notebooks in the context of undergraduate chemical engineering education, starting with a course in statistics.

Undergraduate Training in Statistics

Critical thinking and data analysis are at the core of engineering and scientific training [16, 17]. Statistical analysis provides an objective framework to process and interpret information from data [18]. Despite its relevance, statistical analysis is not necessarily included in all undergraduate engineering curricula [19]. In a recent report [20], ABET states that probability and statistics are to be discussed in engineering curricula to satisfy criteria for accreditation. However, the requirements vary in depth of knowledge and topics to be covered depending on the major [20]. Specifically for chemical engineering, the requirement is to include "applications of mathematics, including differential equations and statistics to engineering problems" [20]. This statement remains too vague and open to the discretion of individual programs. As a result, there is no concerted training and expectations on the degree of knowledge undergraduate chemical

engineering students should acquire in statistical analysis, which may be perceived as lack of training [21].

Many programs incorporate basic concepts as part of their unit operations laboratory modules or have students take a general course in statistics, often offered outside the department. In the latter case, the applications and sample problems are too general or abstract, and chemical engineering students tend to disengage more easily and lose motivation without the direct application of statistics to the profession. Chemical engineering students need robust training in statistical analysis related to risk assessment, process optimization, uncertainty quantification, data modeling, experimental design, and hypothesis testing as an evidence-based and objective approach to process design and understanding as highlighted in the 2022 report *New Directions for Chemical Engineering* by the National Academies of Sciences, Engineering, and Medicine, (Ch 8, 9) [22]. Particularly, instruction for the use of digital data analysis tools to leverage advances in computational power and packages that students can transfer to other areas of their training. There are few chemical engineering programs that address this need explicitly, and no available statistics textbooks or scaffolding materials that focus on the specific needs of undergraduate chemical engineers [23].

Research Goals and Design

This work is the first step in an NSF *Research Initiation in Engineering Formation (RIEF)* study that aims to provide formative mentoring and expertise in pedagogical approaches, qualitative and quantitative data collection, analysis and interpretation, and research-driven design of computational notebooks as scaffolds for undergraduate learning. The research branches from the hypothesis that evidence-based design of computational notebooks can significantly enhance the learning experience and outcomes linked to threshold concepts in an undergraduate statistics course in chemical engineering. In the larger scheme of engineering education, our work will serve to:

- i. select TCs that constitute learning roadblocks in undergraduate engineering statistics courses,
- ii. systematically identify design features of computational notebooks that hinder student learning, and
- iii. use evidence-based design of computational notebooks to scaffold material to facilitate student learning.

We will use *knowledge integration* [24] as the theoretical framework for this study, which is the process of incorporating and synthesizing varied representations resulting in a cohesive body of knowledge. The premise of knowledge integration is that it supports the development of an integrated understanding of a complex domain and can be enabled through the use of technological tools [25]. In this context, students need exposure to instances where they can compare and contrast multiple ideas and representations as part of the instruction [26]. In the case of learning probability and statistics in chemical engineering, we envision that such combinations will be provided through the presentation of applications of relevant statistics concepts in chemical processes and how these affect the actual experimental design to study that process.

Some heuristics to promote knowledge integration have been proposed [27], and we will abide by some of the patterns posed by learning scientists that establish their stages as: (a) eliciting ideas, the stage where students are asked to recall their prior experiences to enrich the learning context, (b) adding new ideas, through meaning-making mechanisms provided to students that enable their ability to make connections between what they know and what is newly presented to them; (c) distinguish ideas, helping them recognizing how the new ideas relate to existing ideas, and identifying any potential conflicts; and (d) sorting out ideas, providing opportunities to refine knowledge [26].

Computational Notebooks

Computational notebooks have become popular in recent years. While computational notebooks were originally focused on strengthening research reproducibility and expanding computational literacy [28, 29], they have now been extensively explored for educational purposes to teach coding fundamentals [30-33], chemical engineering [34-42] concepts (including numerical methods, fluid dynamics, thermodynamics, and kinetics), data science topics [15, 43-46], and other subjects, such as signal processing [47, 48], atmospheric composition [49], optimization [50], and linear algebra [51]. Note that [34] includes a table with detailed annotations for MATLAB and Python-based computational notebooks for chemical engineering specific topics. However, as reported in [52], most literature on the use of computational notebooks for teaching challenging concepts is limited to reporting the implementation of the notebooks, e.g., [48, 50].

The engineering community currently has best practices and common guidelines for the use and content of computational notebooks on various subjects [31]. However, very few studies researched assessments of the learning goals of the courses or concepts summarized by such notebooks, e.g., [53]. Furthermore, fewer endeavors report on outputs related to student experience, such as student engagement [50] or satisfaction [33, 48, 54]. In addition, some criticism exists that computational notebooks can also propagate the dissemination of negative learning outcomes, e.g., poor coding practices [55]. Given these limitations, the focus of this project is on the development of computational notebooks using theory-based design and the evaluation of their effectiveness in the learning of TCs in statistics.

Threshold Concepts (TCs)

Meyer and Land [56] were the first to propose TCs as troublesome yet foundational knowledge in the early 2000's. They proposed the view of TCs as "conceptual gateways" or "portals" that enable access to previously unreachable knowledge. They theorized the characteristics of such as *irreversible* (they are not likely to be unlearned or forgotten), *integrative* (exposing the interrelationships previously hidden on a topic), and *bounded* (has terminal frontiers bordering with thresholds within new conceptual spaces). Examples of threshold concepts include *depreciation* in accounting, *precedent* in law, and *entropy* in physics [57].

Over the past two decades, this definition has evolved into a formal framework in which TCs constitute a learning experience that transforms the understanding of a subject, impacting or creating new ways of reasoning and the ability to explain that knowledge [58]. In this context, the current challenge is to identify discipline-specific TCs as a tool to improve instructor teaching and

course design [11, 59]. Burch et al found lack of curriculum models to identify and overcome TCs; upon discussion of existing models for curriculum development, they propose the conception-focused curriculum (CFC) to help instructors design and deliver courses that enable students overcome TCs [60]. Correia et al present a comprehensive review in [7], and propose a conceptual map to highlight the impact of TCs in instruction and learning processes (see Figure 1).

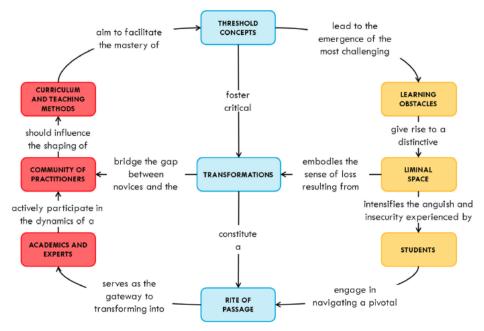


Figure 1 - Correia's conceptual map to show how TCs (blue) impact teaching (red) and learning (orange) and the need to use them to improve teaching approaches (Adapted from the original Figure 1 in [7], by Correia, Copyright (2024), with permission from MDPI Education Sciences, Open Access Creative Common CC BY license)

Threshold Concepts in Engineering

Because of their importance, TCs have been researched in engineering education spaces, including the teaching of specific concepts, such as statics [61], geomatics [8], mechanics of materials [62], and highway design [63]. For example, Atarés et al. investigated how students understand the concept of *entropy* in thermodynamics and proposed that teaching strategies should focus on target conceptual transformation [64]. Their study found that traditional lecture-based approaches fail to address misconceptions caused by students' preconceived notions.

Another study by Davey found that peer presentation is a powerful tool for students to master TCs and should be extended to other engineering courses. The study focused in two core Chemical Engineering courses, i.e. Separations processing and Heat Transfer [65]. For the Separations course, Davey included seven TCs, namely, *equilibrium, two-step equilibrium stage, inverse lever rule, multiple equilibrium stages, net flow, reflux, simplified methods, continuous contact.* Whereas for Heat Transfer, the selected TCs were *theoretical maximum heat energy recovery, practical heat energy recovery, calculation of minimum utility requirements,* and *heat exchanger network representation.* These TCs were identified by a lecturer with 15 years of teaching

experience teaching Separations and another lecturer with 3 years of teaching Heat Transfer, respectively. Davey further examine the TC of *continuous contact* in the Separations course, to examine the relationship between students' self-perceived engagement and their learning of the selected TC. This extended study concluded that student engagement cannot effectively predict the extent of students' understanding of TCs [66].

The University of Western Australia led a national and international discussion on the TCs that first-year engineering students should master as they start their journey to becoming well-rounded engineers, irrespective of their specific discipline [67]. The results were shared in the form of an inventory of TCs for engineers-in-training to guide curricular development and enhancements. Male et al. selected two TCs from the published inventory to further investigate strategies to help first-year engineering students master foundational knowledge to successfully transition into discipline-specific core courses [68]. They focused on the perception and understanding of students on the *role of engineers* and the *value of learning*. The study found that students must get a clear understanding of their future role as engineers in their specific disciplines to motivate their engagement in upper-level courses. These studies highlight current research goals in engineering education to transform the way we teach based on how students learn. More importantly, how to equip instructors to facilitate and guide student learning from quantitative skills to critical thinking and to their role as engineers in society [7, 11, 69].

Some researchers report how TCs were identified and infused into pedagogical practices [70] and to promote specific attitudes in the learners [71]. Nonetheless, most of the work on TCs in engineering rarely reports how the researchers identified the selected TCs [12]. Daugherty et al [72] seek to identify *how* and *what* students learn, they discuss conceptual maps to identify and assess key learning outcomes in engineering courses. Baillie et al. [73] proposed the *threshold capability integrated theoretical framework* (TCITF), which aims to design courses that deeply integrate capability building and knowledge application by combining transformative understanding of knowledge and students' ability to navigate unfamiliar situations. The identification of TCs is not trivial and there is a high potential for the use of TC theories in the development of specific tools for enhancing student learning, particularly those supported by technology. The potential of virtual laboratories to support the understanding of threshold concepts in thermodynamics has been explored [74]. Yet, the potential of being guided through pedagogically involved designs of computational notebooks that should result in student achievement has not been addressed.

Threshold Concepts in Statistics

In the particular case of statistical concepts, some research has explored TCs identified by engineering students and their instructors, leading to the statistics TCs rainbow proposed by Beitelmal et al. [75]. The rainbow, shown in Figure 2, integrates TCs selected by students into the 18 TCs proposed by instructors, to provide the students a more positive learning experience. The rainbow divides statistics concepts into different levels of proficiency analogous to Blooms' taxonomy in which students achieve the next level through demonstrating each set of concepts. Note that this is the only publication that considers statistics TCs in the context of engineering education.

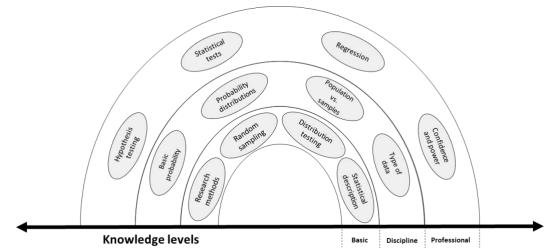


Figure 2. Statistics threshold concepts rainbow as proposed by Beitelman et al. (Adapted from the original Figure 1 in [75] by Beitelmal, Copyright (2022), with permission from MDPI Education Sciences, Open Access Creative Common CC BY license)

Other works have also identified troublesome concepts for students in introductory courses of statistics, albeit in courses geared to Business majors and not in engineering. In 1992, Weaver summarized common topics in which students struggle in statistics, identifying *variability, testing the null hypothesis,* and *confidence interval* [10]. Weaver's piece concludes inviting peer feedback to gather additional examples from daily activities that can help students learn concepts in statistics. In the next two decades, teams around the world started posing the questions we aim to introduce in this review and address in our two-year project: *how* students learn TCs in statistics and how instructors can better scaffold the materials to facilitate the learning process.

Mills, at the University of Alabama at the time of publication, posed the questions of whether computer simulation methods facilitate student learning in statistics [76]. Mills focused on elementary and secondary education, citing common statistics computer software like Excel and MINITAB. Mills examined published work between 1983 – 2000 from social sciences, medicine, business, and statistics education databases among others. Though many researchers advocate for the use of computational tools, little report empirical basis. In [76], Mills discusses the most common statistics concepts for which computational software was employed; the central limit theorem heads the list as simulation experiences allow the student to visualize the shape and sizes of data distributions, and the meaning of sample mean and sampling a distribution. Other concepts for which computational tools were used include *t*-distribution, confidence intervals, binomial distribution, regression analysis, and hypothesis testing. Though initially intended as an exploration for basic concepts in statistics, Mills also covers advanced topics that are certainly relevant for undergraduate and graduate engineering students, like Bayesian statistics, regression analysis, and Analysis of Variance (ANOVA). Written at the beginning of the 2000s, Mills' review also recognizes that access to the internet plays a key role for both instructors and students. However, technological tools also open the space for misconceptions if there is no appropriate feedback and monitoring during student learning.

Dunne et al at the University of Cape Town (UCT), published their experience teaching statistics in higher education in the 2003 Conference Proceedings issue of the International Association of Statistical Education [77]. Their work aimed to identify TCs in basic statistics by surveying students taking their second semester of undergraduate statistics in Business majors. 465 students, 25% of the class enrollment at UCT, were asked to explain in their own words random sample and the central limit theorem as well as list three concepts they found the simplest and the most difficult in their first semester of introduction to statistics. Some concepts appeared in both the "simplest" and "most difficult" categories, Dunne et al decided this divergence in student opinion was worth using to identify such concepts as potential TCs: probability, chi-square distribution and test, ttest, Poisson distribution, F-test, binomial distribution, normal distribution, and regression analysis. These results led the team to introduce innovations to the first semester statistics curricula; for example, computer simulation was introduced to facilitate learning of sampling distribution. Dunne reports improvement in student learning and no identified drawbacks; however, the team acknowledged that computer literacy may be a factor that deserves further examination [77]. Finally, the authors emphasize the relevance of selecting the appropriate textbook according to discipline-specific requirements; the team considered 12 possible textbooks for their introduction to statistics course for Business majors. Notably, there is an urgent need for a statistics textbook that specifically addresses the interests of students in chemical engineering [23].

A final contribution we discuss here is Khan's study to identify TCs in first-year business statistics [9]. By 2014, Khan still emphasized the lack of research on TCs in mathematics and statistics, especially on *how* to TCs and implement them in curriculum development. Khan discusses previous work done to identify statistics TCs for biology and business majors, acknowledging that a few students from science and engineering would enroll in said courses, but constituted the minority of enrollment. A discussion on methods used to identify TCs lists phenomenographic interviews, questionnaires, student surveys, short problems, and review of examination scripts as common alternatives [9]. The TCs identified in this work include *random variables, expected values, chi-square, actual vs expected frequencies* (chi-square tests). The author concludes with implementations in course design guided by the selected TCs.

A common point across the works cited in this review is that discussion among discipline experts is key in identifying TCs as well as student feedback collected over multiple semesters. We hope this work will serve as a catalyst for discussion among peers teaching introductory courses in statistics to engineering students, particularly in Chemical Engineering. As this project evolves, we intend to expand the conclusions from this work to other courses in Chemical Engineering as well as other engineering disciplines.

Proposed Threshold Concepts in Statistics for Chemical Engineers

In agreement with the TCs identified by Beitelman et al. [75], and heavily aligning with the first author's experience while teaching introduction to statistics in previous years the following two TCs were selected for the current study:

Sample vs. population [75-77]

Students struggle to make a clear distinction between samples and populations; therefore, they do not make correct use of appropriate formulas and test statistics during the semester's in-class activities, homework, quizzes, and final exam. This is particularly evident when selecting the appropriate probability distribution to use in building confidence intervals or performing hypothesis tests. The goal of the computational notebook to be developed around this threshold concept will be to give students guided feedback as they work through decision trees that will impact the final answer and interpretation if sample and population are not understood correctly.

Random variables [9, 75]

Starting on week 4 of the semester, students use random variables to describe outcomes of a random experiment, select the appropriate probability distribution to model data based on the nature of the experiment at hand, combine random variables, determine the uncertainty of the property of interest, build confidence intervals, and carry out hypothesis tests. It is, therefore, of critical importance students can determine and define, in words, the random variable in a specific setting. Another computational notebook will be developed to teach this threshold concept.

Students' experience and expected challenges

Anonymous surveys to undergraduate students in the chemical engineering statistics course at our university during the Fall 2023 and 2024 terms showed that nearly 25% of the class struggled with "identifying outcomes of experiments," and over 40% with "operations with events." Currently, this course has reading assignments prior to covering the content in the classroom. These assignments come with built-in adaptive questions to track student performance. Interestingly, student engagement and satisfaction with textbook reading during the said semesters varied widely. The class was also asked for feedback on the use of computational tools to consolidate learning of key concepts, students found coding troublesome and that it impedes their learning. It is important to recognize that many factors influence the perceived adequacy of the course material. For example, students may not dedicate enough time to assimilate the reading material, or students may attempt the review questions multiple times until selecting the correct answer without paying attention to the reading. Similarly, students may not dedicate enough time to review the sample coding material, or students may still have questions related to the concept at hand that prevents them from using coding tools to solve the problem. We recognize that the computational notebooks we will be creating will provide an alternative to students to navigate deficiencies they perceive in currently available materials.

Discussion

From the explored literature we can conclude that TCs have previously been explored both in chemical engineering and statistics independently. However, the intersection of statistics education for chemical engineers has not been investigated yet, highlighting the value of the project here introduced. Our inquiry will harness existing knowledge in TCs in both areas and will use theoretically sound approaches for the design of computational notebooks targeting the learning of such TCs. In particular, the two TCs that will be first used in this project (Samples vs Population, and random variables) were confirmed as part of those reported by Baillie et al. [57] as gathered through their Delphi study of TCs for introductory statistics courses.

Through this literature review we also identified the common approaches used to identify TCs in both, statistics and chemical engineering, which relies heavily on the opinion of experts, often experienced instructors in their areas [50, 56]. This highlights an area of opportunity for this project, as we are planning to start our inquiry with two TCs that the first author identified in her own practice teaching statistics for chemical engineers. However, we could further contribute to the identification of more TCs by consulting the community of practitioners at the intersection of statistics and chemical engineering to find collective agreement on these and more TCs, adding validity to this inquiry and opening new spaces for future research.

Finally, this literature review also helped advancing our understanding on the latest theoretical developments that have taken place in the space of TCs. Enhancing our understanding of valuable newly proposed frameworks such as the threshold capability integrated theoretical framework (TCITF) [57] which could support the development of our project and the design of the envisioned computational notebooks in synergy with pedagogical theories such as the computational cognitive framework [2, 18] which is currently part of our research design.

Conclusions and Future Work

This work-in-progress paper has provided a brief review of the literature related to teaching undergraduate statistics for chemical engineers, computational notebooks for educational use, and threshold concepts broadly and specifically for engineering and statistical concepts. It constitutes a solid foundation and with new theoretical insights that can strengthen the design and execution of the described project and course design in general.

The next stages of this project involve the design and development of the planned computational notebooks followed by their use and evaluation during the Fall 2025 semester. Further inquiries related to the identification of TCs might be part of the new research agenda derived from this review and project outcomes. For instance, utilizing computational notebooks for additional TCs, theoretical explorations, and/or further innovations in the development of computational notebooks as well as course design of the statistics course in our department.

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