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Original Article

Complementary role of large language models in educating undergraduate design of distillation column: Methodology development

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ABSTRACT

This paper explores the integration of large language models (LLMs), such as ChatGPT, in chemical engineering education, departing from conventional practices that may not be universally accepted. While there is ongoing debate surrounding the acceptance of LLMs, driven by concerns over computational instability and potential inconsistencies, their inevitability in shaping our communication and interaction with technology cannot be ignored. As educators, we are positioned to play a vital role in guiding students toward the responsible, effective, and synergetic use of LLMs. Focusing specifically on distillation column design in undergraduate mass-transfer courses, this study demonstrates how ChatGPT can be utilized as an auxiliary tool to create interactive learning environments and simulate real-world engineering thinking processes. It emphasizes the need for students to develop critical thinking skills and a thorough understanding of LLM principles, taking responsibility for their use and creations. While ChatGPT should not be solely relied upon, its integration with fundamental principles of chemical engineering is crucial. The effectiveness and limitations of ChatGPT are exemplified through two case studies, showcasing the importance of manual calculations and established simulation software as primary tools for guiding and validating engineering results and analyses. This paper also addresses the pedagogical implications of integrating LLMs into mass transfer courses, encompassing curriculum integration, facilitation, guidance, and ethical considerations. Recommendations are provided for incorporating LLMs effectively into the curriculum. Overall, this study contributes to the advancement of chemical engineering education by examining the benefits and limitations of LLMs as educational aids in the design process.

Introduction

Chemical engineering education has traditionally focused on imparting fundamental knowledge, equipping students with a strong theoretical foundation (Goedhart et al., 1998; Molzahn and Wittstock, 2002). However, in today's rapidly evolving technological landscape, there is increasing recognition of the importance of bridging the gap between theoretical concepts and real-world applications through practical problem-solving experiences (Crosthwaite et al., 2006; Liebmann, 1956; Wisniak, 1998). Recent advancements in chemical engineering education have emphasized the integration of computer software, coding skills, and software tools such as Aspen Plus, Simulink, MATLAB, and Python into the curriculum (Rahman et al., 2013; Sunarso et al., 2020). These tools empower students to tackle realistic industrial problems, cultivate Industry 4.0 skills, and enhance their core understanding of chemical engineering principles (Moodley, 2020). Moreover, in the midst of this evolving technological landscape, we are witnessing the increasing presence and influence of advanced language models like ChatGPT.

The acceptance of ChatGPT into the education landscape, spanning various fields such as engineering, chemistry, and sciences, has been a subject of robust debate. This debate arises mainly due to the computational instability and the notorious potential for generating

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Nomenclature

Abbreviation

AI	Artificial intelligence
GA	Genetic algorithms
LLM	Large language models
NRTL	Non-Random Two-Liquid
PSO	Particle swarm optimization
SA	Simulated annealing

inconsistent or erroneous results, in particular *[the computational stability of LLMs model is unreliable]* and *[employing ChatGPT in tasks that involve complex computations most probably will generate inconsistent or erroneous results]* (Reviewer 1, 2023; Reviewer 2, 2023). Tyson (2023) reported that ChatGPT can be bad at maths. Nonetheless, it is inevitable that these models will eventually become an integral part of our lives, shaping the way we communicate and interact with technology. It is highly likely that students, the young and future generation, have started utilizing these models, irrespective of their current limitations in generating consistent and accurate results. As educators, we find ourselves in a position where we cannot control the presence or usage of ChatGPT, but we can play a vital role in educating students on its responsible and effective utilization. Clark (2023) concludes that *[ignoring this technology may be unwise and a more prudent approach would be to continue to monitor its capability and adapt assignments as the technology improves]*. In this context, we turn to a common and fundamental task, i.e., design of distillation columns, as our representative case study and we aim to vividly exemplify how LLMs like ChatGPT can play a pivotal role in enhancing the learning experience for students in the field of chemical engineering. Nonetheless, it is worth noting that ChatGPT models have also found application in other areas of chemical engineering, such as protein modeling (Mann and Venkatasubramanian, 2021), crystallization (Sitapure and Kwon, 2023a), and metal-organic framework research (Kang et al., 2023).

Chemical engineers, in their jobs, are anticipated to be able to design and/or develop a distillation system or unit for separating the individual components from the liquid mixtures based on their boiling points, sometime in small scale and at other times in large scale. In line with the emergence of ChatGPT, the main objective of this paper is to demonstrate how we can educate students, particularly those in engineering disciplines, to responsibly use ChatGPT as an effective auxiliary tool to create an interactive learning environment and simulate real-world engineering thinking processes, specifically in distillation column design. Students must develop critical thinking skills and a thorough understanding of the principles behind language models, taking responsibility for their use and creations. It is essential to recognize that we cannot solely rely on ChatGPT and instead, it must be used together with the fundamental principles of chemical engineering and other relevant sciences. By leveraging upon the capabilities of ChatGPT, we seek to explore its potential in making the students obtain initial insights and rules of thumb, question the design process, and enable them to engage with advanced technology. Manual calculations and established simulation software remain essential and necessary as the main verifying tools to guide and obtain sound and appropriate engineering results and analyses. Our goal is to use the differences that may arise between ChatGPT-generated designs and manual calculations to trigger questions and further explorations. Hence ChatGPT plays a key role in encouraging students from various engineering and scientific disciplines to critically evaluate the outputs and exercise judgment in incorporating them into their decision-making processes. Through this approach, we empower students to harness the benefits of ChatGPT while remaining cautious and cognizant of its limitations.

Through presenting case studies and examples, we aim to demonstrate how ChatGPT achieves these aforementioned roles and how it can be effectively applied to engineering students. Alongside the benefits, we will also address the challenges associated with ChatGPT, including the current computational limitations and the need for further research to improve its reliability and accuracy performance in complex calculations. By embracing the presence of ChatGPT as part of our educational landscape, we can prepare students for a future where responsible and informed usage of these advanced technologies is essential whilst making the educators updated and relevant on the powers and limitations this technology brings into the engineering and scientific education landscape.

In the following sections, we will present two case studies that exemplify the application of ChatGPT in a chemical engineering problem-solving context. These case studies demonstrate how ChatGPT can provide an alternative approach to distillation column design and showcase the differences that arise between ChatGPT-generated designs and manual calculations. Through these examples, we also outline the common challenges faced when using ChatGPT as an aid in distillation column design, emphasizing the importance of understanding the underlying principles. By providing examples and highlighting key considerations, we aim to equip Professors and students with the necessary knowledge to use ChatGPT effectively in conjunction with manual calculations and benchmark simulation software.

Methodology

This section presents the methodology employed to explore the application of ChatGPT as an aid in distillation column design, including the steps involved in case study selection, utilizing ChatGPT for design parameter suggestions, validation, and verification using Aspen Plus, and addressing the challenges and critical considerations in integrating ChatGPT with manual calculations. The framework is graphically represented in Fig. 1.

1. **Identification of case studies:** The first step involves identifying relevant case studies that are available in the literature. From these case studies, we will extract important mixtures and separation criteria, including feed flowrate, feed composition, distillate purity, and bottom purity. In addition, the physical chemistry property (i.e., thermodynamic data) should be extracted from the literature. For simplicity's sake, as our target audience is undergraduate students, we will limit our analysis to conventional distillation systems for the separation of binary mixtures.
2. **Utilizing ChatGPT for design parameter suggestions:** Once we have gathered the necessary case studies, including the established

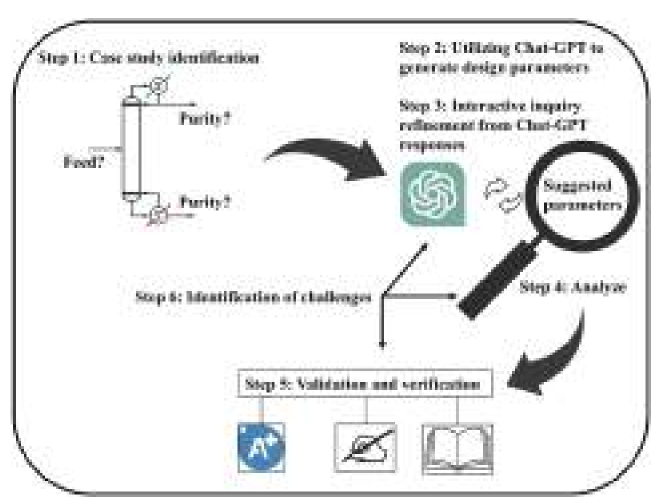

Fig. 1. Framework employed in this work.

designs and corresponding design parameters such as feed stage location, number of trays, reflux ratio, reboiler duty, and the thermodynamic packages, we will leverage ChatGPT to suggest design parameters to achieve the specified separation requirements. Importantly, we will not provide ChatGPT with the design parameters from the existing studies. Instead, we will rely on ChatGPT to provide us with its suggestions.

3. **Interactive inquiry refinement from ChatGPT responses:** The ChatGPT will provide a general response with typical design steps after the first simple inquiry as someone without any background, in which, initial insights for further inquiry improvement could be sought. Moreover, several critical assumptions, correlations, and rules of thumb can be collected from ChatGPT responses. The information can be iteratively accumulated into the subsequent inquiry for better ChatGPT responses. Fig. 2 depicts the general iterative inquiry algorithm. A sample of the interactive inquiry refinement from ChatGPT responses will also be provided in Section 3.1 for educational purposes.
4. **Analyze ChatGPT's calculation:** After receiving the suggested design parameters from ChatGPT, we will further engage with the model to understand its decision-making process and request it to show us the calculations behind its recommendations. We will meticulously record the calculation steps provided by ChatGPT.
5. **Validation and verification:** This step is of paramount importance as it involves validating and verifying the design suggestions obtained from ChatGPT. For chemical engineering students, one can utilize Aspen Plus, a widely recognized process simulation software, to simulate the proposed designs and assess their feasibility and effectiveness. If the suggested designs yield satisfactory results, chemical engineering students can confidently compare the simulation outcomes with the established literature found in Step 1. Additionally, they can perform manual design calculations based on their engineering knowledge and expertise, and then compare their results with those suggested by ChatGPT. This comprehensive approach ensures a two-fold verification process, strengthening the validity of the obtained designs. Alternatively, manual design calculations can be conducted, which may require a basic understanding of engineering principles. If the initial design suggestions do not meet the desired separation requirements, they will continue an iterative process with ChatGPT, seeking further suggestions until a suitable solution is obtained. Subsequently, they can compare the final design solution with established literature and the manual calculations conducted.
6. **Identification of challenges and key considerations:** Throughout the methodology, we will discuss the common challenges encountered when utilizing ChatGPT as an aiding tool in distillation column design. Emphasis will be placed on the importance of understanding the underlying principles and considerations necessary to effectively integrate ChatGPT with manual calculations. By addressing these challenges and providing key considerations, this work aims to

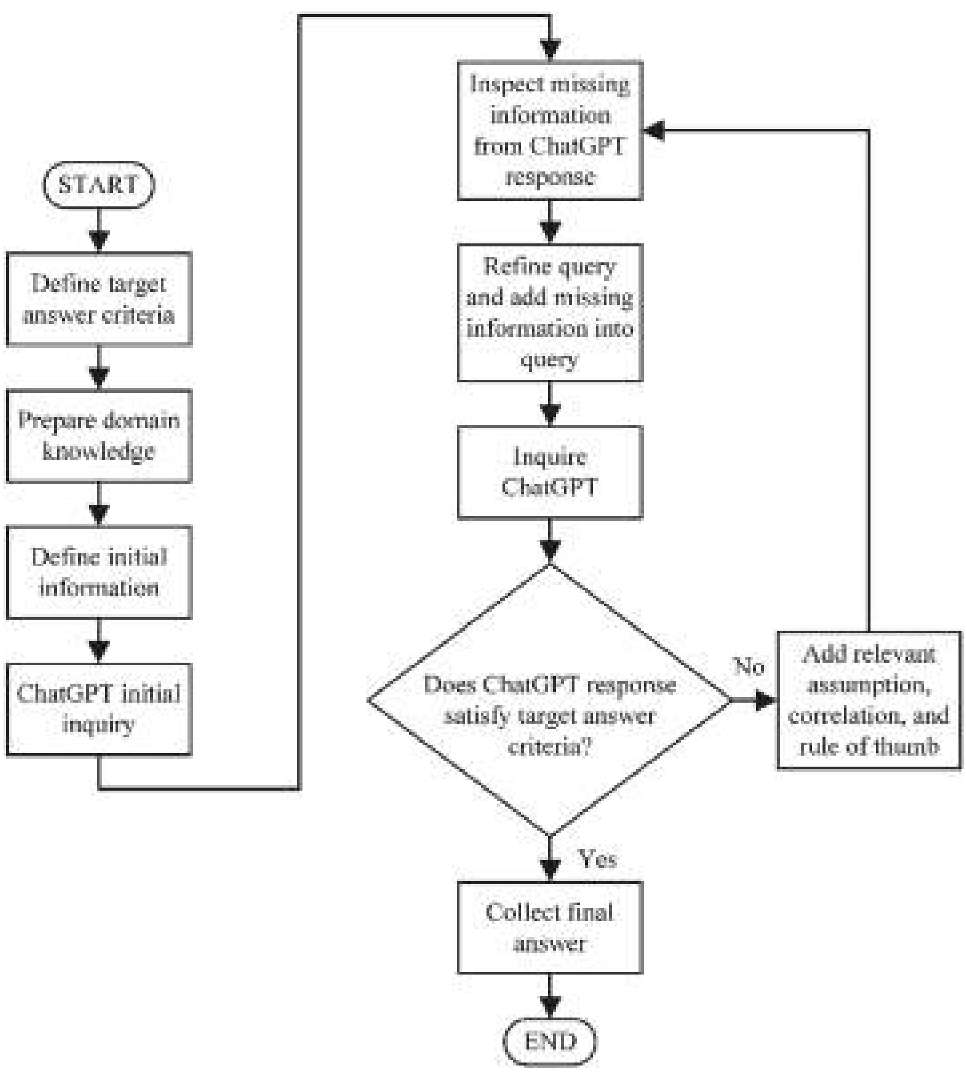

Fig. 2. Iterative inquiry algorithm.

enhance student learning in mass transfer courses at the undergraduate level. The utilization of ChatGPT as an educational tool in distillation column design not only provides students with hands-on experience but also fosters a deeper understanding of mass transfer principles, preparing them for success in their mass transfer coursework.

Note, however, that for such a framework to be implemented into undergraduate courses, it is essential for students to have a basic understanding of mass transfer principles and chemical engineering fundamentals. For the detailed implementation, it is recommended to introduce the potential application of ChatGPT as an aiding tool for designing distillation columns only at a later stage in the mass transfer course, ideally during the second half of the semester. This sequence allows students to develop a solid understanding of mass transfer before utilizing ChatGPT as an aid in their design process. While previous exposure to process simulation software like Aspen Plus is beneficial, it is not mandatory for implementing the validation and verification step in this methodology.

While our work does not involve the creation of a standalone LLM model (e.g., "DistillationGPT" or "SeparationGPT") or substantial enhancements to existing LLM models (e.g., GPT-3 or GPT-3.5), it is important to highlight that our primary objective centers on demonstrating the practical application of ChatGPT, a readily available language model, in the context of undergraduate chemical engineering education. We wish to reiterate that our goal is to highlight the pivotal role that ChatGPT can play in educating students on its responsible and effective utilization. This approach addresses a pressing need in the current educational landscape, where the effective and responsible integration of AI technologies into pedagogy is a critical concern.

Case studies

Case study 1: separation of n-heptane and isobutanol

In this case study, we draw upon the work of Luyben (2017) as a reference for the separation of n-heptane and isobutanol (Fig. 3**(a)**). This choice was made with the aim of providing a simplified scenario that is suitable for our target audience of undergraduate students. By focusing on a relatively straightforward separation process, we can effectively demonstrate the application of ChatGPT as an educational aid in distillation column design. The feed stream has a flowrate of 100 kmol hr^{-1}, with equimolar components. The separation goal is to achieve a product purity of 99.9 mol.% for both the distillate and the bottoms. To obtain a distillation column design that fulfills these requirements, we input this relevant information into ChatGPT using the following command "*Suggest an atmospheric distillation column design for 100 kmol/hr and 50 mol.% n-heptane/isobutanol feed, to achieve 99.9 mol.% top and bottom products concentration. I know this can be complex but at least please suggest the proper design and proper design parameters, for example, feed location, number of trays, reflux ratio, diameter of column, flooding factor, etc. Also, please calculate the top and bottom product condition. Please help to suggest a suitable thermodynamic package for this separation*". Based on this input, ChatGPT generates the total number of stages, feed location, reflux ratio, and suggested an appropriate thermodynamic package, which can be subsequently used in Aspen Plus for simulation purposes. **Figure S1** presents a snapshot of the response generated by ChatGPT, and Fig. 3**(b)** illustrates the resultant flowsheet simulated using Aspen Plus. It should be noted that the response shown in **Figure S1** was obtained after an iterative refinement process, which is not depicted here due to the cluttered nature of the full chat conversation. To demonstrate the interactive inquiry refinement, a new sample conversation was constructed for Case 1, as presented in **Table S1 (Supporting Information)**. It is important to acknowledge that the suggested parameters from ChatGPT may vary, as seen in **Figure S1** and **Table S1**, as ChatGPT's responses are not always identical. For this reason, it becomes crucial to emphasize to students the significance of conducting manual calculations to obtain accurate and reliable engineering results and analyses. Encouraging students to critically evaluate the outputs and exercise judgment in incorporating them into their decision-making processes is paramount. Through this approach, we empower students to harness the benefits of ChatGPT while maintaining a cautious and mindful approach, fully aware of its limitations. **Table S1** provides an illustrative example of the iterative process, while the suggested solutions were based on an earlier conversation during the project's initiation. Note that some suggestions by ChatGPT may work while others may not. In cases where the suggested solution does not yield the desired results, it is necessary to continue the iterative process with ChatGPT for further suggestions until a suitable solution is achieved. A specific example of such a situation is presented in Case 2.

The comparison between the simulated flowsheet in Fig. 3**(b)** and the specifications set for the distillate and bottoms products reveals notable differences. Interestingly, both the distillate and bottom purities achieved using ChatGPT are significantly higher, reaching 99.99 mol.%, surpassing the target of 99.9 mol.%. As a consequence, there is a remarkable increase in both the condenser and reboiler duty, with a percentage increase of 43 and 34 %, respectively. Moreover, the reflux ratio suggested by ChatGPT deviates noticeably from Luyben's work. It is considerably higher, indicating a greater emphasis on reflux in ChatGPT's design recommendation. In terms of column configuration,

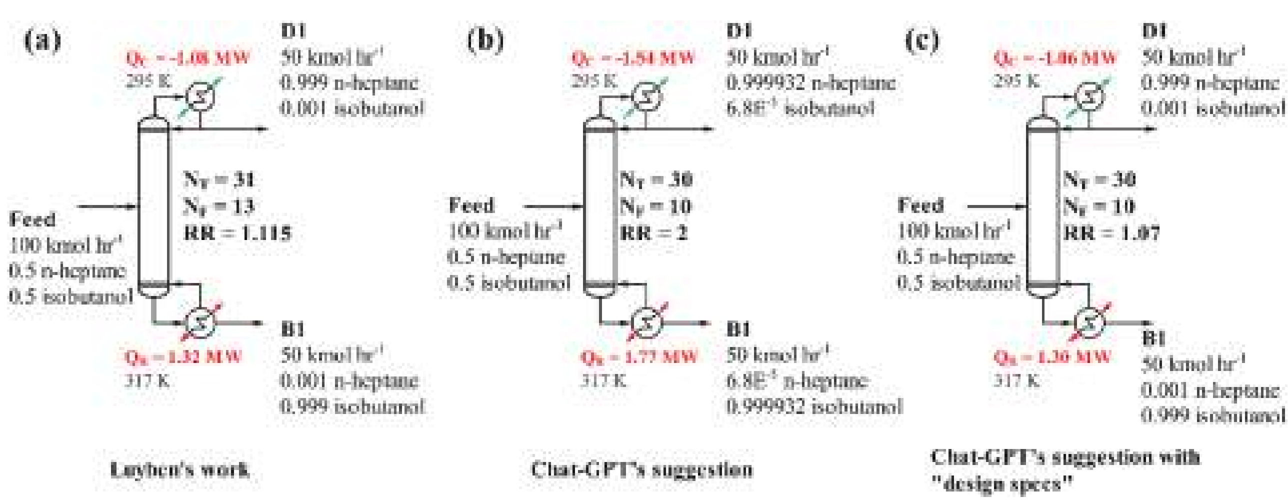

Fig. 3. The simulated configuration using Aspen Plus for Case 1: (a) Base case reproduced from (Luyben, 2017), (b) ChatGPT's suggestion, and (c) ChatGPT's suggestion with activated design specs.

there is a close agreement between ChatGPT's suggestion of 30 stages (Fig. 3**(b)**) and Luyben's simulation of 31 stages (Fig. 3**(a)**). The feed stage locations also exhibit close proximity, with ChatGPT proposing the 10th stage and Luyben utilizing the 13th stage in his simulation. To ensure a fair and meaningful comparison between the two flowsheets, we believe that this can be achieved through activating the design specifications feature in Aspen Plus to fix the top and bottom purities at the desired value (Fig. 3**(c)**). From Fig. 3**(c)**, it can now be seen that the top and bottom product purities are set to the specification value of both at 99.9 mol.%. Upon comparing the results obtained from Luyben's work (Fig. 3**(a)**) and that using ChatGPT with activated design specs (Fig. 3**(c)**), it becomes evident that both flowsheets are quite similar, with minor differences in the number of stages, feed stage location, reboiler duty, condenser duty, and reflux ratio only. Regarding the thermodynamic package, ChatGPT initially suggested the Non-Random Two-Liquid (NRTL) model, which differs from those used by Luyben (2017). However, upon prompting, ChatGPT admitted it was a mistake and proposed using the UNIQUAC model instead.

In addition to comparing the results generated by ChatGPT with literature work, additional verification can be made by validating the design *via* manual calculation. Fig. 4 illustrates the xy diagram for n-heptane and isobutanol obtained through manual calculations using the McCabe-Thiele method. The steps involved in the manual design can be found in Fig. 5. The total number of stages was found to be 16, and the feed location is at the 4th stage (Fig. 4). These parameters are then input into Aspen Plus, resulting in the column configuration shown in Fig. 6 **(a)**. Upon comparing Fig. 6**(a)** to Fig. 3, it becomes apparent that the design generated through manual calculations falls short of achieving the desired purity separation. The purity of n-heptane and isobutanol at the distillate and bottom only reaches 99.6 mol.%, slightly lower than the specified value of 99.9 mol.%. Additionally, there is a significant increase in the reboiler and condenser duties, attributed to the lower number of stages in the manual design compared to those obtained through ChatGPT and Luyben's work. A lower number of stages generally results in higher energy consumption for the system. To ensure

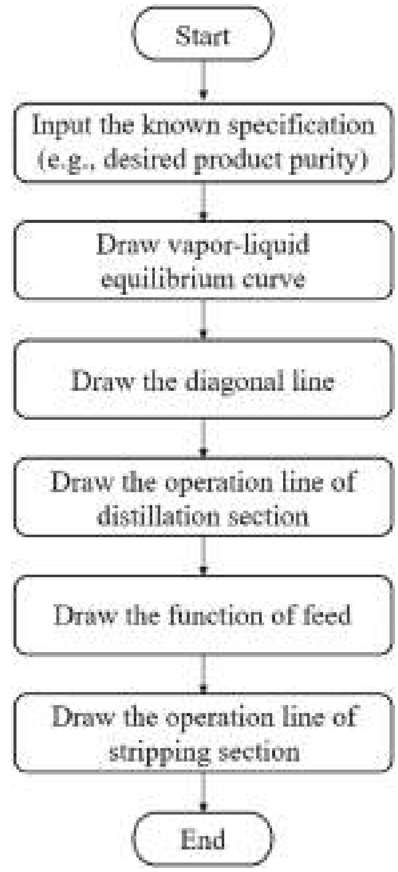

Fig. 5. Steps for manually designing distillation column.

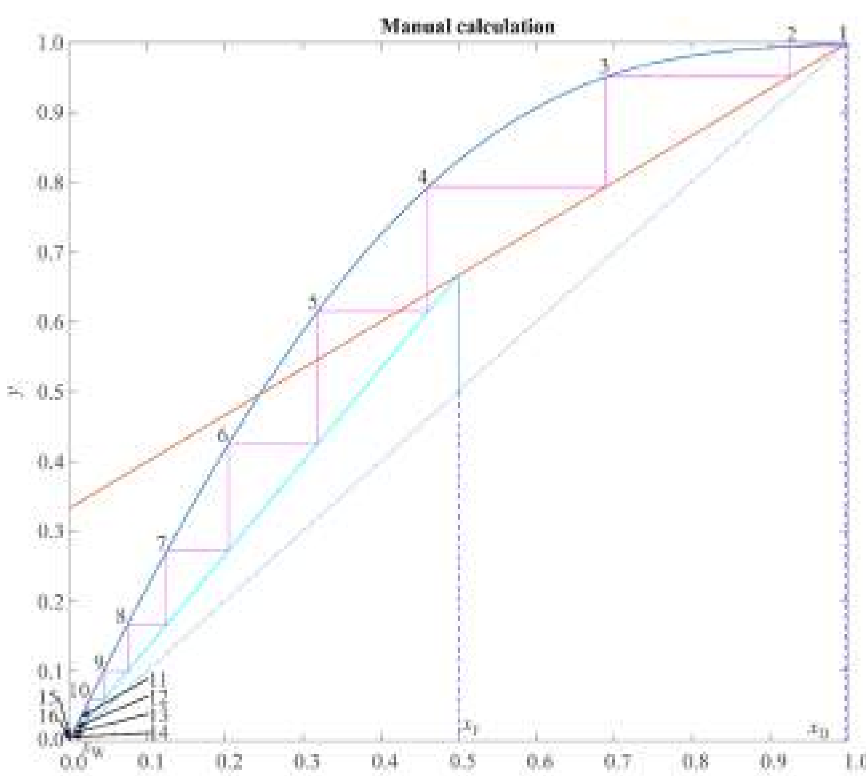

Fig. 4. Manual design for binary separation of n-heptane and isobutanbol using McCabe-Thiele method.

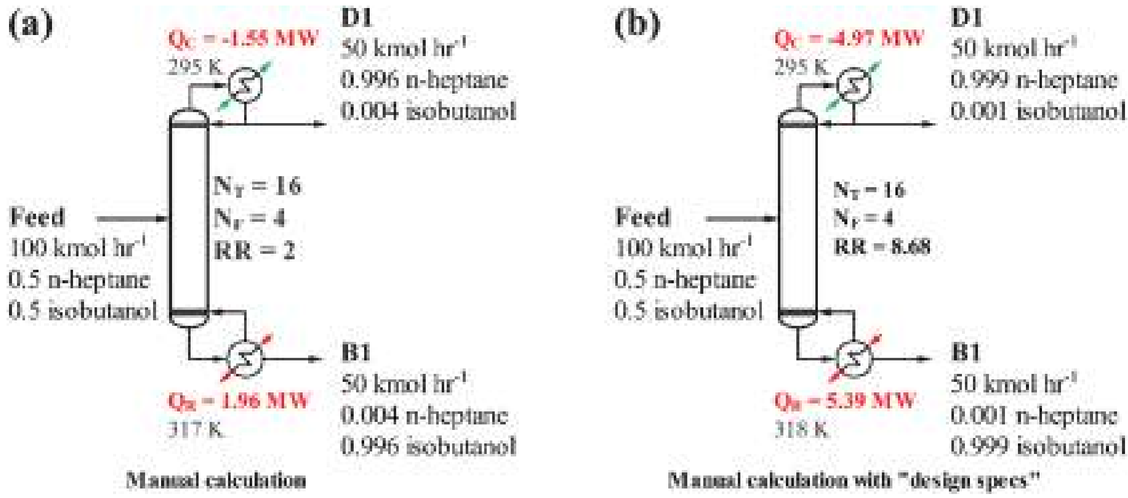

Fig. 6. The simulated configuration using Aspen Plus for Case 1: (a) manual calculation and (b) manual calculation with activated design specs.

consistent comparison, the design specifications feature in Aspen Plus can be activated to fix the top and bottom purities at 99.9 mol.%. The resultant flowsheet is depicted in Fig. 6**(b)**. Upon comparing Fig. 6**(b)** to Fig. 3, it becomes clear that the reflux ratio, as well as the reboiler and condenser duties, experience a significant increase. This can be attributed to the same reason mentioned earlier, where the manual design generates a lower number of stages compared to the designs obtained through ChatGPT and Luyben's work. A lower number of stages typically leads to higher energy consumption in the system.

Overall, this case study demonstrates the significant potential of ChatGPT in aiding the design of distillation columns, particularly in the context of mass transfer courses for undergraduate students. It demonstrates that while ChatGPT may not generate identical designs as those obtained through manual calculations, it offers valuable suggestions

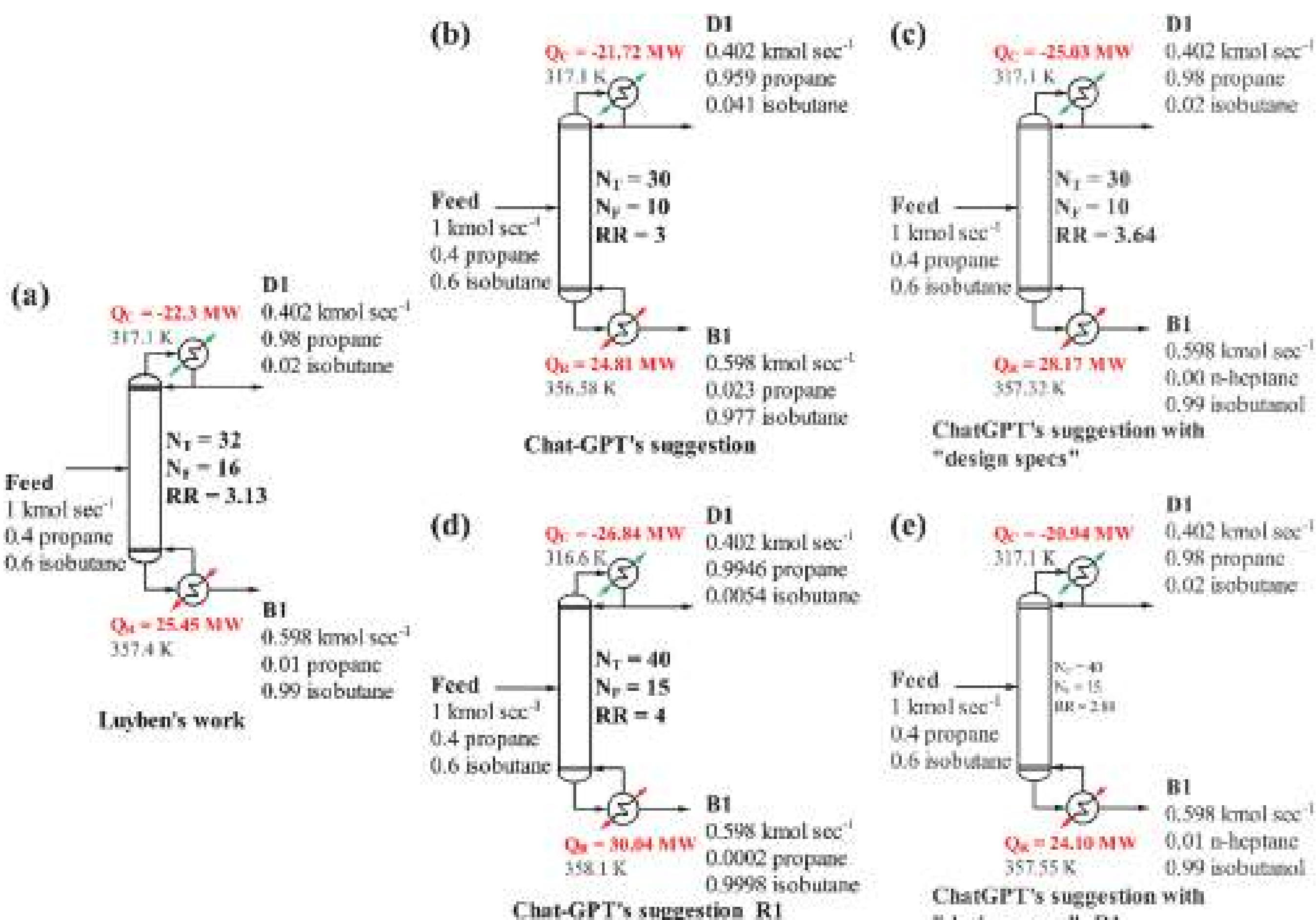

Fig. 7. The simulated configuration using Aspen Plus for Case 2: (a) Base case reproduced from Luyben (2013), (b) ChatGPT's suggestion, (c) ChatGPT's suggestion with activated design specs, (d) Chat-GPT's suggestion Revision#1, and (e) ChatGPT's suggestion Revision#1 with activated design specs.

that facilitate the generation of initial designs with ease. This is particularly advantageous compared to the tedious and time-consuming process of manual calculations using methods like McCabe-Thiele. While it cannot guarantee a design that meets all separation requirements, ChatGPT allows for an iterative process by inputting commands or utilizing the design specification feature in Aspen Plus. It is important to emphasize that both the designs provided by ChatGPT (Fig. 3**(b)** and Fig. 3**(c)**) and the manual calculation (Fig. 6) may not be optimal. However, establishing these initial flowsheets is a crucial step toward further optimization and obtaining the optimum column configuration. It is essential to note that this case study focuses solely on the initial design phase and does not delve into the exploration of subsequent optimization processes (i.e., constraint handling).

Case study 2: separation of propane and isobutane

The second case study is also based on the work of Luyben (2013), which serves as a reference for guidance in setting up steady-state simulations in Aspen Plus. This book has been a valuable resource, especially for beginners in the field of process design and control. Similar to Case 1, the selection of this case aims to provide a simplified example that is well-suited for our target audience of undergraduate students. By focusing on a relatively straightforward separation process, we can effectively showcase the application of ChatGPT as a powerful educational tool in the design of distillation columns.

Fig. 7**(a)** illustrates the configuration for a simple binary separation of propane and isobutane, as described by Luyben (2013). The feed stream consists of 1 kmol sec^{-1} with a composition of 40 mol.% propane and 60 mol.% isobutane. The objective is to achieve a distillate purity of 98 mol.% propane and a bottoms purity of 99 mol.% isobutane. To obtain a distillation column design that meets these requirements, we followed the identical method demonstrated in the previous case study, inputting the relevant information into ChatGPT using the following command "*Suggest a trayed at 14 atm distillation column design for 1 kmol/sec containing 40 mol.% of propane and 60 mol.% of isobutane, to achieve 98 mol.% top product of C3 and 99 mol.% bottom product of C4. I know this can be complex, but please suggest the proper design parameters, such as feed location, number of trays, reflux ratio, diameter of column, flooding factor, etc. Also, please calculate the top and bottom product conditions. Also, please calculate the top and bottom product condition*". Note that the purpose of using 14 atm here is to ensure a reflux drum temperature of around 325 K or 52 °C, which enables the use of inexpensive cooling water in the condenser instead of costly refrigerants. Similar to the previous case, ChatGPT generates the total number of stages, feed location, reflux ratio, and suggested an appropriate thermodynamic package based on this input, which can subsequently be used in Aspen Plus for simulation purposes.

The resultant simulated flowsheet is depicted in Fig. 7**(b)**. One significant observation was that the top and bottom product purities are much lower than the specification (Fig. 7**(b)**). The distillate product for propane barely reaches 96 mol.% while the bottom product for isobutane barely reaches 98 mol.%. This appears to be different from Case 1 where both the parameters suggested by ChatGPT provides significantly higher distillate and bottoms purities, reaching 99.99 mol.%, surpassing the target of 99.9 mol.%. Of course, it is possible for one to try activate the design specifications feature that is made available in Aspen Plus to fix the top and bottom purities at the desired value. In some cases, this may work and some may not. If it works, one should expect the duty to be higher since the column specification generated by ChatGPT provides product purities much lower than the desired specification. Fig. 7**(c)** reflects such scenarios and the fact that for this particular case, one can fix purities using the column parameters provided by ChatGPT by simply activating the design specification. Note that this may not be always the case. Another possible alternative is to continue an iterative process with ChatGPT, seeking further suggestions until a suitable solution is obtained. The following command is inserted "*Earlier on, I asked to suggest a 14 atm distillation column design for 1 kmol/sec containing 40 mol.% of propane and 60 mol.% of isobutane, to achieve 98 mol.% product of C3 and 99 mol.% bottom product of C4. I know this can be complex but at least please suggest the proper design and proper design parameters, for example, feed location, number of trays, reflux ratio, diameter of column, flooding factor, etc. Also please calculate the top and bottom product condition. The results you provided are as below: Feed Location: Place the feed on the 10th tray from the bottom of the column. Number of Trays: Start with a preliminary estimate of 30 trays. This number can be adjusted based on the separation requirements and optimization results. Reflux Ratio: Set the reflux ratio to 3:1 (3 mol of liquid reflux per mole of distillate). Diameter of Column: Use a column diameter of 1.5 m. Operating Pressure: The column operates at 14 atm. Unfortunately, the top and bottom products can only reach 95.9 mol.% and 97.7 mol.%, respectively, after I input your suggested parameters into Aspen Plus. Could you please check and re-suggest column parameters that can achieve 98 mol.% product of C3 and 99 mol.% bottom product of C4?*".

Subsequently, ChatGPT provided an alternative suggestion for the design parameters, leading to a revised flowsheet depicted in Fig. 7**(d)**. Notably, ChatGPT proposed an increase of 10 stages in the total number of stages and shifted the feed location downward by 5 stages. Additionally, the reflux ratio was suggested to increase from 3 to 4. As a result, the bottom purity significantly increased to 99.98 mol.%, surpassing the target of 99 mol.%. Similarly, the distillate purity reached 99.46 mol.%, exceeding the desired specification of 98 mol.%. Consequently, there was a remarkable increase in both the condenser and reboiler duty, with a percentage increase of 20 and 18 % with respect to Luyben's work (Fig. 7**(a)**). To ensure consistency in the comparison, we can employ the same approach as in the previous section, activating the design specifications feature in Aspen Plus to fix the top and bottom purities at their desired values. Fig. 7**(e)** illustrates this adjustment. The top and bottom product purities are now set to their specified values of 98 mol.% and 99 mol.%, respectively.

Upon comparing the results obtained from Luyben's work (Fig. 7**(a)**) and the initial suggestion provided by ChatGPT (Fig. 7**(b)**), a couple of notable distinctions become apparent. Firstly, ChatGPT's initial design displays a reduction of 2 total stages in comparison to Luyben's configuration. Furthermore, a substantial divergence of 6 stages is observed in terms of the feed tray location between the two flowsheets. The reboiler and condenser duties deviate from Luyben's design by only 3 %, which we consider acceptable. Moreover, the reflux ratios are quite comparable, with the ChatGPT design requiring a slightly higher reflux ratio. When comparing the results obtained from Luyben's work (Fig. 7 **(a)**) and the alternative suggestion provided by ChatGPT (Fig. 7**(d)**), it becomes apparent that ChatGPT suggests a larger number of stages. This could be attributed to the initial suggestion from ChatGPT not meeting the desired product specifications and, in a humorous sense, "afraid" of the consequences, leading to an increase in the number of stages. However, the feed location remains relatively similar, which is also in close proximity to Luyben's design. On the other hand, the condenser and reboiler duties of the alternative design deviated significantly from Luyben's design, reaching up to 20 %. Regarding the thermodynamic package, ChatGPT suggested the UNIQUAC model, which is consistent with thos reported by differs from those used by Luyben (2013).

Fig. 8 presents the xy diagram for the propane and isobutane mixture obtained through manual calculations using the McCabe-Thiele method. The procedure followed in this case is identical to Case 1, and the steps can be found in Fig. 5. The manual calculations reveal that the total number of stages is 30, with the feed location at the 14th stage. These parameters are then input into Aspen Plus, resulting in the column configuration depicted in Fig. 9**(a)**. Upon comparing Fig. 9**(a)** with Fig. 7 **(a)**, it becomes evident that the design generated through manual calculations also falls short of achieving the desired purity separation, analogous to Case 1. The propane purity at the distillate only reaches 97 mol.%, slightly below the specified value of 98 mol.%. Likewise, the isobutane purity at the bottom only reaches 98 mol.%, lower than the

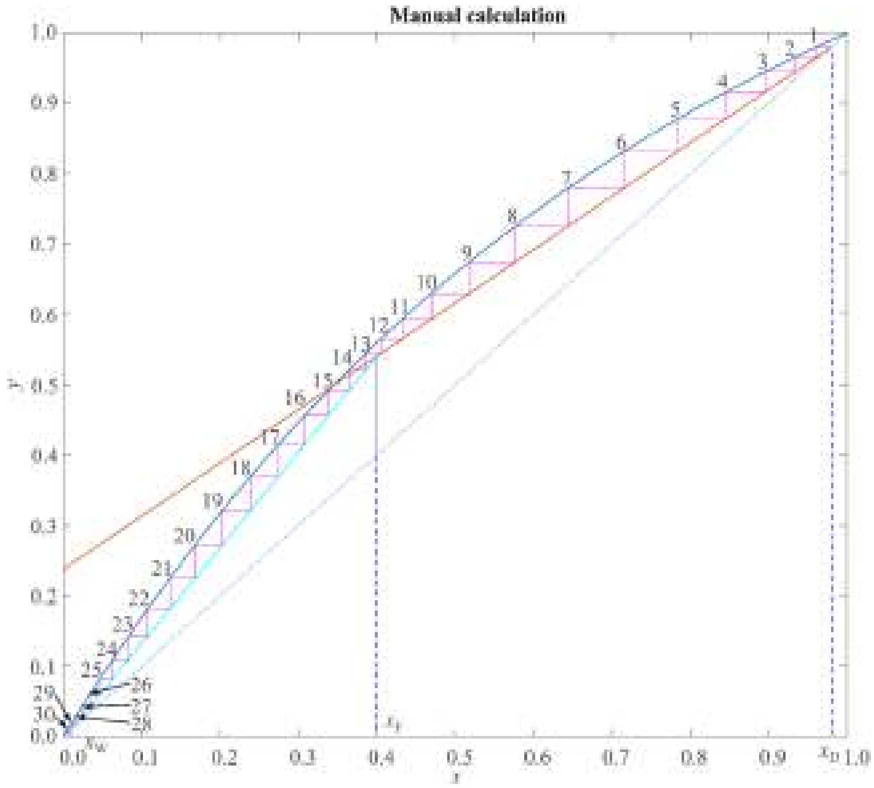

Fig. 8. Manual design for binary separation of propane and isobutane using McCabe-Thiele method.

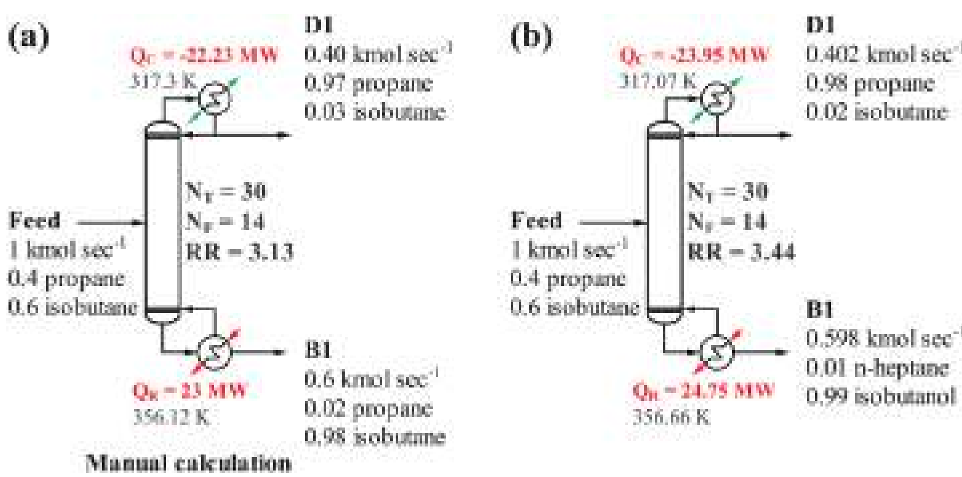

Fig. 9. The simulated configuration using Aspen Plus for Case 2: (a) manual calculation and (b) manual calculation with activated design specs.

desired value of 99 mol.%. This discrepancy can be attributed to the significantly lower reboiler duty in the design generated through manual calculation (Fig. 9**(a)**) compared to the literature design (Fig. 7 (a)). In contrast to Case 1, it is interesting to note that the design obtained through manual calculations in this case provides the same number of total stages and feed location, albeit to a slightly different extent. To ensure consistent comparison, the design specifications feature in Aspen Plus can be activated to fix the top and bottom purities at their desired values. The resulting flowsheet is depicted in Fig. 9**(b)**. Upon comparing Fig. 9**(b)** with Fig. 7**(a)**, it becomes clear that the design closely resembles the literature design, with only a small difference observed in the reflux ratio and condenser duty. This variation can be attributed to the slight disparity in the total number of stages and feed location between the manual calculation and literature design.

In summary, this case study further underscores the significant potential of ChatGPT as a valuable tool for aiding the design of distillation columns, particularly within the context of mass transfer courses for undergraduate students. Building upon the previous case study, it highlights the importance of an iterative process with ChatGPT, where further suggestions are sought until a suitable solution is obtained. It is crucial to emphasize that the flowsheets generated by ChatGPT can serve as an “initial design” for subsequent process optimization and the attainment of the optimum column configuration. In fact, on a slightly more advanced level, if undergraduate students are expected to design a plant under optimal conditions, Aspen Plus and MATLAB can be integrated to perform optimization using algorithms such as Particle Swarm Optimization (PSO) (Yang et al., 2023b), Genetic Algorithms (GA) (Kong et al., 2023), and Simulated Annealing (SA) (Yang and Ward, 2018). The design proposed by ChatGPT serves as the initial design for process optimization. During the optimization step, the MATLAB optimization algorithm relies on this initial flowsheet to iterate and determine the optimum configuration based on objective functions like the total annual cost (TAC) and design constraint and boundary. Our previous works have exemplified such a methodology, which can be referred to by interested readers (Kong et al., 2022a, b; Yang et al., 2023a, 2022a, b).

Depending on the assignments or tasks assigned to undergraduate students, they can and should tailor their commands to ChatGPT and utilize the suggestions generated by ChatGPT appropriately. However, it is crucial to reemphasize that blind reliance on ChatGPT's suggestions should be avoided, and manual calculations should always be incorporated to verify ChatGPT's suggestions. In this work, a two-fold verification process is employed, where the design suggestions obtained from ChatGPT are validated against established literature, and manual design calculations are performed to compare the results with those suggested by ChatGPT.

By doing the inquiry iteration (**Table S1**), students can learn what is required by ChatGPT to obtain the specific target. ChatGPT response can provide the general approach for distillation column design and students can specify several targets for the improvement of ChatGPT response on the next iteration. ChatGPT may also need to use specific correlations, assumptions, and rules of thumb where students can include or ask ChatGPT for self-implementation. Computational details can also be demanded onto ChatGPT so that specific values can be obtained for further verification. With the interactive iterative approach, specific refinement can be executed properly and systematically. The overall iterative procedure may be executed in at least 5 iterations or even less if clear instructions are given. We use the free ChatGPT 3.5 in this work to show that everyone can utilize the same tools without financial burden, i.e., pay for advanced ChatGPT 4 or higher, to obtain relatively good insights for the preliminary design of the distillation column. Moreover, with good domain knowledge, the response of ChatGPT can be refined accordingly, i.e., the calculations of hydraulic constraints, tray flooding, and pressure drop, which require detailed tray design, tray spacing, tray hole diameter, downcomer design, and other hydraulic parameters.

Pedagogical implications

The integration of artificial intelligence (AI) technologies, such as ChatGPT, into undergraduate mass transfer courses holds significant potential for transforming the way students learn and engage with complex topics like distillation column design. By leveraging upon the power of AI, students can benefit from enhanced learning experiences.

Using ChatGPT as a learning tool provides students with access to a virtual tutor that offers immediate explanations, clarifies concepts, and provides additional examples and resources. This interactive and personalized learning experience allows students to grasp the intricacies of distillation column design more effectively. Engaging with ChatGPT encourages students to think analytically about distillation column design. The model prompts students to evaluate different design alternatives, assess trade-offs, and justify their decisions based on underlying principles. This promotes a deeper engagement with the subject matter and cultivates students' abilities to evaluate, synthesize, and communicate engineering concepts effectively.

While AI technologies like Chat-GPT offer numerous benefits, it is crucial to recognize the role of instructors in facilitating effective integration and ensuring optimal learning outcomes. Instructors play a pivotal role in the following areas:

- **Curriculum integration**:

Instructors should carefully integrate ChatGPT into the undergraduate curriculum, aligning it with course objectives and learning outcomes. They should identify suitable learning activities, assignments, and assessments that leverage the capabilities of the AI model while complementing traditional teaching methodologies. It would be appropriate to task undergraduate students using ChatGPT to generate a design, simulate it in Aspen Plus to ensure its functionality, and then perform a final verification using manual calculations. This approach ensures that students do not blindly rely on ChatGPT but instead understand the importance of manual calculations in mass transfer, enabling them to develop sufficient skills as they progress to higher levels. By pinpointing the reasons behind any discrepancies between the results from manual calculations and the solution suggested by ChatGPT, students can enhance their understanding of mass transfer principles.

- **Facilitation and guidance:**

Instructors play a vital role in guiding students and providing appropriate supervision when incorporating AI tools like ChatGPT in the classroom. This involves setting clear expectations, monitoring students' progress, and offering timely feedback to foster meaningful interactions. They can facilitate discussions on the limitations and assumptions of AI models, encourage analysis of AI-generated results, and emphasize the importance of manual calculations for comprehensive learning. By striking the right balance between AI tools and traditional methods, instructors can help students harness the benefits of AI while nurturing their analytical skills and promoting a deeper understanding of engineering and scientific principles. Instructors can also provide additional explanations or supplementary materials to complement the AI-generated responses, ensuring a balanced learning experience.

- **Ethical considerations:**

Instructors must address ethical considerations associated with AI integration in education. This includes discussing the limitations of AI models, addressing potential biases or inaccuracies in responses, and promoting the responsible use of AI tools. By reinforcing evaluation of the AI-generated outputs, instructors can teach students to question and verify information when necessary, promoting ethical awareness, and responsible use of AI technologies. Additionally, instructors should familiarize themselves with legal requirements related to data privacy, intellectual property, and fair use when incorporating LLMs in the classroom. This ensures that students' rights and privacy are protected and that the use of LLMs complies with legal frameworks and institutional policies.

- **Continuous improvement:**

Instructors should actively seek feedback from students regarding their experience with ChatGPT. This feedback can help identify areas for improvement and inform future iterations of the AI model or the instructional approach. Instructors should also stay updated on the latest advancements in AI and adapt their teaching strategies accordingly.

For the curriculum design that integrates ChatGPT into undergraduate (i.e., specifically mass transfer for Chemical Engineering) courses, the following recommendations are proposed:

- **Delivery:**

As indicated briefly in **Section 2**, it is recommended to introduce the potential application of ChatGPT during the second half of the mass transfer course, allowing students to develop a solid understanding of mass transfer principles before incorporating ChatGPT into their design process. The delivery can include three two-hour computer laboratory sessions. In the first session, an overview of ChatGPT and the methodology introduced in this work can be provided, which covers the process from case study identification (Step 1) to validation and verification (Step 5). It is assumed that students taking this course have prior experience with Aspen Plus from prerequisite modules. However, if necessary, additional lab sessions can be made available to refresh or introduce basic Aspen Plus tutorials to the students. The second session should guide students on how to appropriately use ChatGPT to design distillation columns for case studies, following the methodology introduced in this work. The last session can be a practice session where students are given additional open-ended case studies without the configuration, requiring them to work independently. The instructor can move around the lab to check on each student's progress. Pairing students in groups during this session can facilitate collaboration, allowing them to work together alongside ChatGPT and fostering bonds for future assignments.

For students who are new to Aspen Plus and have limited engineering knowledge, it is essential to include two or three additional lessons that offer a concise introduction to basic manual calculations. These supplementary lessons will equip them with the necessary knowledge and skills to confidently participate in the process.

Such an approach provides students with the necessary background knowledge and hands-on experience to effectively utilize ChatGPT as a valuable tool in their distillation column design process.

- Assignment/Tasks:

For the graded assignment, it is recommended to engage students in a small design project for distillation column design, where they can utilize ChatGPT as a powerful tool for generating initial design parameters and apply their knowledge of mass transfer principles to perform manual calculations for verification.

Additionally, for researchers, ChatGPT can be a valuable tool for generating initial designs, particularly when time constraints limit extensive manual calculations and simulations. In the context of optimization, conducting manual calculations may not be necessary as the solution provided by ChatGPT serves as the initial solution, and parameters can be adjusted during the optimization process to yield the optimum solution. This integration of ChatGPT supports the iterative design process and can be used in conjunction with optimization algorithms. However, it is crucial to maintain a balance by incorporating manual calculations and verification to ensure a thorough understanding of mass transfer principles and develop a holistic approach to distillation column design in both educational and research contexts.

Future directions

The integration of ChatGPT into undergraduate mass transfer courses has opened up exciting possibilities for further research and development in the field of AI-assisted distillation column design education. As educators and researchers continue to explore the potential of ChatGPT, several areas can be developed to improve its implementation and expand its capabilities within the curriculum.

Integration with virtual simulations:

Researchers can explore the integration of ChatGPT with virtual simulation platforms to provide students with a more immersive learning experience. By coupling ChatGPT with simulation software, students can not only generate design solutions but also visualize and evaluate their performance in a virtual environment.

Collaboration and peer learning:

Future research can focus on incorporating collaborative features into ChatGPT, allowing students to work together in groups or engage in peer learning activities. By enabling students to interact with ChatGPT collectively, they can exchange ideas, compare design strategies, and collectively evaluate the generated solutions. This collaborative aspect promotes teamwork and communication, essential for successful engineering practice.

Assessing student learning and performance:

To ensure the effectiveness of ChatGPT in mass transfer courses, future research can explore methods for assessing student learning and performance when utilizing the model. This involves developing appropriate assessment metrics and rubrics that capture the holistic understanding and problem-solving skills acquired through the interaction with ChatGPT. By evaluating the impact of ChatGPT on students' learning outcomes, researchers can refine the implementation and identify areas for improvement.

To be more specific in assessing students' learning and performance, we recommend educators to design problem-solving assignments that necessitate students to use ChatGPT as a tool to propose solutions for particular engineering problems. These assignments can assess their capacity to apply the solutions provided by ChatGPT to real-world scenarios, taking into consideration factors such as feasibility, efficiency, and safety. Another avenue for assessment involves assigning projects in which students compare the recommendations given by ChatGPT with those derived from conventional engineering methods. This assesses their ability to evaluate and substantiate the distinctions or similarities between these approaches. Furthermore, educators can create simulation-based exercises utilizing software like Aspen Plus or similar process simulation tools. Students can be tasked with simulating distillation processes based on both ChatGPT's suggestions and traditional methods, with assessments centered on their capability to set up and accurately interpret simulation results. Lastly, long-term projects that require students to use ChatGPT at various stages, from problem formulation to final design, can be assigned. Assessments for these projects can evaluate students' ability to incorporate feedback and iterative improvements into their projects, thus providing a comprehensive view of how ChatGPT influences their learning and performance in mass transfer courses. This multifaceted assessment approach allows educators to gauge students' knowledge and practical application of engineering principles alongside AI-powered tools.

Ethical considerations and responsible use:

As ChatGPT becomes more prevalent in undergraduate mass transfer courses, it is crucial to address the ethical considerations and responsible use of AI technologies. Future research should focus on exploring the ethical implications of ChatGPT usage, addressing issues such as biases, transparency, and privacy concerns. Developing guidelines and best practices for instructors and students to ensure responsible and ethical utilization of ChatGPT is paramount.

Specialized GPT models for distillation:

Another particularly promising avenue for future research lies in the development of dedicated GPT models designed explicitly for distillation. These specialized models can be build upon the foundation of the extensively pretrained GPT-3 backbone, a feat already achieved in several recent studies (Chronopoulou et al., 2019; Liévin et al., 2022; Sitapure and Kwon, 2023b). By adopting a domain-specific fine-tuning approach and leveraging the wealth of knowledge and data resources available in the context of distillation, researchers can meticulously craft GPT models that excel in tasks unique to the field of distillation. These specialized models combine the expansive general knowledge characteristic of GPT-3 with finely tuned expertise in addressing the intricate challenges specific to separation science. The result is a potent educational and practical tool, poised to enhance distillation column design education for both students and professionals, offering tailored, high-precision support for their endeavors.

Conclusion

In conclusion, the application of LLMs such as ChatGPT into undergraduate education has the potential to revolutionize the teaching and learning process. By leveraging upon advanced natural language processing capabilities, ChatGPT can serve as a powerful tool for designing distillation columns in mass-transfer courses. Through interactive and collaborative activities, students can enhance their understanding of distillation column design principles while gaining valuable hands-on experience with advanced technology. While ChatGPT streamlines the design process, it is important to emphasize the foundational knowledge and manual calculations. The presented case studies demonstrated the benefits of using ChatGPT as an aiding tool while acknowledging the need for verification through established literature and widely used simulation software. The pedagogical implications suggest the active role of instructors in curriculum integration, facilitation, ethical considerations, and continuous improvement to ensure optimal learning outcomes. Overall, the utilization of AI technologies like ChatGPT in chemical engineering education holds promise for transforming the learning experience and preparing students for success in the modern chemical engineering landscape. The authors plan to test this concept in the upcoming mass transfer course at Sunway University Malaysia and the process design course (4287) at National Chung Hsing University offered to chemical engineering undergraduates in September 2023. Feedback will be collected and analyzed, with results to be published in a follow-up manuscript tentatively scheduled for the first half of 2024. This study aims to determine the effectiveness, appropriateness, student preferences, and academic value of integrating ChatGPT into the course. For future work, we also suggest exploring the potential of integrating ChatGPT into batch distillation or flash distillation scenarios. These topics hold significant relevance to undergraduate education and can contribute to a comprehensive understanding of distillation and separation processes, offering students a more holistic perspective on the subject.

Data availability statement

All data generated or analyzed during this study are available from the corresponding authors upon reasonable request.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

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