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The Use of Artificial Intelligence in Capstone Design Courses

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Integrating AI-Based Polymer Design Tools into a Chemical Engineering Capstone Course

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Abstract

The use of artificial intelligence (AI) in both classrooms and workplaces has grown significantly in recent years. Students who lack education and experience in AI risk being left behind in this technological revolution. Therefore, it is more important than ever for students to be equipped with the knowledge and skills to effectively use AI and understand its impact. In response to this growing need, several lectures were delivered in a chemical engineering capstone design course offered at the University of Arkansas which exposes students to two AI and machine learning tools developed at Georgia Tech — Polymer Genome (PG) and PolyBERT (PB). The goal was to show how these AI and machine learning tools can assist in polymer processing and in predicting or understanding general polymer properties. The lectures were divided into several sections, including understanding the differences between AI and machine learning; learning how to use Polymer Genome and PolyBERT; comparing results from these tools to more general AI software such as ChatGPT; and exploring real-world applications of the PG and PB software. To demonstrate student learning, the students completed a short polymer project that incorporated the use of the software tools in real-world scenarios. Surveys were used to assess student interest and the effectiveness of this activity. Generally, the students thought that this brief introduction to the use of AI gave them something they could talk to employers about when asked the question "tell me what you have done with AI." They also found it useful that AI could allow them to design polymers to be used in ASPEN simulations. Although the technology was used in the capstone design project, it could be equally used in many other classes such as polymer processing, materials, or even fluids. We plan to make course content available upon request for anyone that wants to build on this approach.

Introduction

While it is widely recognized that artificial intelligence (AI) use and innovation have accelerated rapidly in recent years, there remains limited formal education on how to effectively interpret and apply AI-based tools. This gap is particularly evident in university classrooms, where the role of AI continues to be actively debated as its accessibility and popularity increase. However, AI adoption is not limited to academia; its use in industry is also expanding rapidly. Recent industry reports indicate that 78% of companies use AI in at least one business function, highlighting its growing importance in technical careers [1].

It is estimated that by 2025, approximately 50% of the global workforce will require reskilling due to AI integration, up from 41% in 2023 [2]. This rising demand for reskilling underscores the consequences of limited AI literacy and emphasizes the need for structured educational approaches that prepare students to engage effectively with AI-driven technologies. In today's highly competitive and evolving job market, career readiness is a fundamental objective of higher education and integrating guided AI strategy in educational frameworks institutions can equip students with skills needed for the modern engineering era [3,4]. With AI becoming increasingly embedded in engineering practice, it is critical to equip the next generation of engineers with the skills needed to understand, evaluate, and responsibly use AI tools.

Most educators and students are now familiar with widely used AI tools such as ChatGPT, Grok, Google Gemini, and Microsoft Copilot, and many have begun to recognize both the strengths and limitations of these platforms. There is little doubt that such tools can be thoughtfully integrated into the classroom when used appropriately. However, these general-purpose AI systems are not designed specifically for engineering applications and often lack the technical depth and accuracy required to address specific engineering concepts. As a result, their ability to provide reliable insight into specialized engineering problems is limited.

As these general and convenient AI models have grown, so has the creation of engineering specific AI models. PolyBERT and Polymer Genome are two polymer-specific AI models that have been developed in recent years to predict properties of both known and novel polymers. To help students develop a stronger understanding of AI and AI-based tools relevant to engineering practice and future careers, several lectures were incorporated into a senior-level chemical engineering capstone course. An additional goal of these lectures was to teach students how to effectively analyze results from these AI-based software tools and critically assess the accuracy of the predictions using their engineering knowledge. Following the lectures, the students were assigned a project using the two programs and a post survey was conducted to assess student learning. A pre-course survey was not administered, as the initial intent of the project was instructional implementation rather than formal publication, and therefore baseline data on students' prior familiarity with AI tools was not collected.

Each group had complete freedom to determine their capstone project and had the option to incorporate AI-based tools into their work. The only major requirement for the project is they must use Aspen Plus and Capcost for analysis of their process. Of all the groups, only one used a polymer in their project. This group (6 students) attempted to utilize Polymer Genome to gather the necessary information for their Aspen Plus simulations but ultimately found an easier method to collect the information directly within Aspen. Therefore, the AI-polymer project was designed as a standalone instructional activity intended to expose all students to engineering-specific AI tools, regardless of their primary capstone topic.

PolyBERT and Polymer Genome

Polymer Genome is an online polymer informatics platform developed by Ryan Lively and Rampi Ramprasad at the Georgia Institute of Technology. The platform enables on-demand prediction of a wide range of relevant polymer properties using machine-learning models trained on high-throughput density functional theory (DFT) calculations and experimental data from the literature and existing databases [5]. These models establish quantitative relationships between polymer structural features and macroscopic properties, allowing rapid property estimation without the need for additional experiments or simulations.

For accessibility, Polymer Genome is implemented as a web-based tool comprising three primary modules: homopolymers, copolymers, and the diffusion lab. In the homopolymer and copolymer modules, users input polymer structures using the Simplified Molecular Input Line Entry System (SMILES), a standardized text-based representation of chemical structures. These modules output predicted thermal, mechanical, and physical properties depending on the polymer chemistry, with each prediction accompanied by an estimated uncertainty.

The diffusion lab module differs substantially from the homopolymer and copolymer sections. This module employs machine-learning models specifically trained to predict solvent solubility and gas permeability/selectivity in polymer materials [6]. In addition to a polymer SMILES string, the diffusion lab requires a SMILES representation of the solvent, along with solvent activity, and solvent density. Based on these inputs, the platform predicts diffusion coefficients and solvent sorption values, enabling evaluation of polymer–solvent transport behavior.

Together, these three modules provide access to a diverse set of polymer properties relevant to materials design and engineering applications. Because Polymer Genome is delivered as a web-based interface, the learning curve for new users is minimal, with the primary requirement being familiar with SMILES notation for polymer structures.

The second program covered in the class was PolyBERT, which was also developed by Lively and Ramprasad. PolyBERT enables fully end-to-end machine-driven polymer informatics that uses artificial intelligence methods [7]. PolyBERT is a program that uses Python. The code is free to the public and can be accessed online. The base code for PolyBERT cannot by itself predict polymer properties, but when a linear regression model is added to the code, specified properties can be predicted. Since PolyBERT requires working in Python and modifying code, the initial learning curve is steeper than with Polymer Genome. In return, PolyBERT is more flexible and can be applied to a wider variety of polymer property predictions.

Lecture Content

As part of a chemical engineering capstone course, four lectures were dedicated to this material. The first lecture served as an introduction to artificial intelligence and machine learning while also establishing a foundational understanding of polymer science, as many students had not previously taken a polymer-focused course. Before the lecture, students indicated they were confident in using general AI tools but did not know of specific engineering AI tools. Real-world examples of polymer processing from our research laboratory were presented and discussed to aid in the students' understanding of the material. Students were educated on some of the challenges associated with polymer processing and why understanding certain properties of polymers are important. Various common AI software tools were presented, and students were asked to discuss the pros and cons of each software tool. Lastly, the students learned about the emerging importance of AI and the use of AI for engineers in the workplace.

The second lecture focused on the Polymer Genome (PG) platform. This lecture covered the underlying principles of how PG operates and provided practical examples demonstrating how to use the software and interpret its predicted material properties. All three modules of the Polymer Genome platform—homopolymers, copolymers, and the diffusion lab—were presented and discussed in the context of their real-world applications. One example from the diffusion lab involved assessing whether a specific polymer would be a suitable membrane material based on its diffusion behavior with varying gases. After each module, the instructor and students discussed the generated results to assess whether the predictions were reasonable, using fundamental chemical engineering principles to interpret the results.

The third lecture was based on the software polyBERT. In this lecture students were introduced to the underlying concepts of how polyBERT works, at least to the degree of understanding what was required to use the program. The objective of the lecture was not to teach the students Python or Visual Studio code; therefore, this portion of the lecture was kept brief. Students followed the instructions and walked through how to install the Python and Visual Studio codes. The students were provided with a base PolyBERT code template and guided through each section of the code to understand its function and role in generating property predictions. Students were then shown how to use the code to predict tensile strength and melting temperatures of different polymers. Lastly, the students were taught the advantages and limitations of polyBERT.

The final lecture compared the two platforms, Polymer Genome and PolyBERT, highlighting their respective strengths and limitations. The discussion also addressed how students could use these tools to obtain polymer property data and incorporate the data into Aspen Plus simulations. This was intended to support students whose capstone projects involved polymers modeled in Aspen Plus.

Project Content

To evaluate the students' understanding of the two software platforms, a short project was assigned. The project consisted of three main sections: short-answer questions, a section using Polymer Genome, and a section utilizing PolyBERT. For the Polymer Genome section, questions focused on utilizing the homopolymer and diffusion lab features of the platform. In the PolyBERT section, students were primarily tasked with modifying the provided code to predict specific properties, such as tensile strength, and implementing their own enhancements to the model. Students were also required to analyze and evaluate the accuracy of the resulting predictions. While some questions had definitive correct answers, most were intentionally open-ended, allowing students to explore the tools in a self-directed manner and apply their prior chemical engineering knowledge to assess the model predictions.

Survey Results and Discussion

To assess the impact of the lectures and the project and gather feedback for future improvement, a post survey was developed. The survey was distributed to students after the class was finished for the semester. Out of the 41 students in the class, 22 responded, resulting in a 53.6% participation rate. The survey was divided into three main sections: Polymer Genome, PolyBERT, and feedback on the lectures and project. The first two sections of the survey were formatted as statements beginning with 'I understand…,' and students responded using a 1–5 scale, where 1 indicated strong disagreement and 5 indicated strong agreement with the statement. Additionally, some questions in the first two sections were phrased as 'How likely are you…,' with responses again recorded on a 1–5 scale, where 1 indicated very unlikely and 5 indicated very likely.

Section 1: Polymer Genome

The students first indicated their level of understanding of Polymer Genome and its methodology for estimating polymer properties, as illustrated in Figure 1. Among the 22 participants, an average rating of 3.68/5 suggests that the lectures effectively introduced students to how Polymer Genome works, especially given that most students had no prior familiarity with the software. While the majority of students rated their understanding as 3 or higher, a small number selected a rating of 1, suggesting that the instructional impact was not entirely consistent across all participants. This group that rated their understanding as 1 may be influenced by their previous experience with computational tools and AI-based property prediction methods. Overall, these results indicate that most students gained a solid understanding of Polymer Genome's methodology for estimating polymer properties.

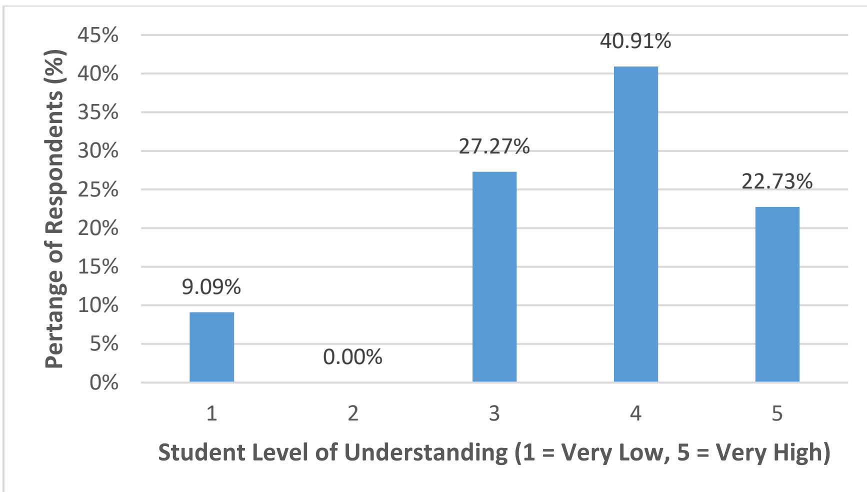

Figure 1. Survey Results Showing Student Understanding of Polymer Genome after Instructional Lectures (average = 3.68/5, n = 22).

The next survey question assessed the students' understanding of the advantages and disadvantages of Polymer Genome. As is seen in Figure 2 students reported a mean rating of 3.95/5, suggesting a level of agreement that they understood both the benefits and limitations of the software from the lecture material. While the average rating suggests that most students reported moderate to high levels of understanding, a smaller subset (approximately 15%) indicated limited understanding, selecting ratings of 1 or 2. This variation may reflect differences in exposure to AI based tools or different perspectives students have on AI driven tools, specifically Polymer Genome in this case. The results from this survey question suggest that further description of the advantages and disadvantages in future lectures could be beneficial to students.

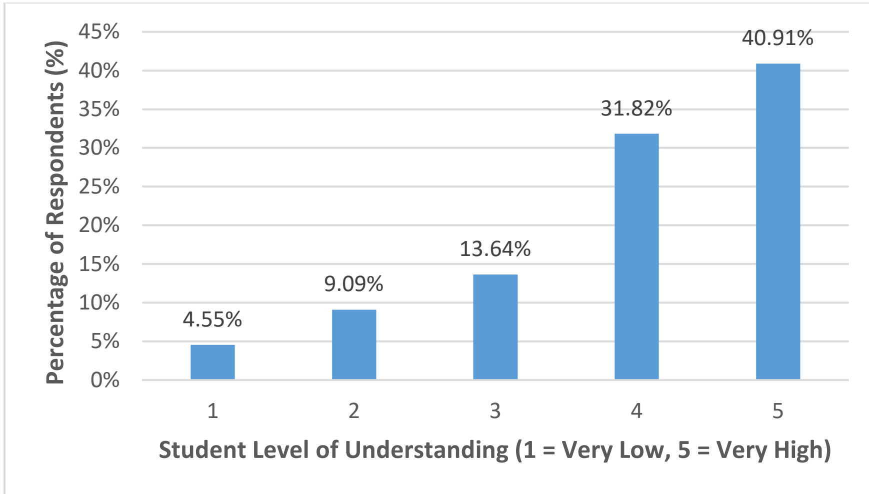

Figure 2. Survey Results Showing Students Understanding the Advantages and Disadvantages of Polymer Genome (average = 3.95/5, n = 22).

Students were next asked to rate their understanding of how Polymer Genome could be applied in industry. Figure 3 shows an average response of 4.18/5, indicating the students felt that they had a strong understanding of how Polymer Genome could be used beyond the classroom and how it could add to their overall engineering skillset. This result demonstrates the effectiveness of the lectures.

Following this, the students were asked how likely they were to use Polymer Genome in future classes, with the results shown in Figure 4. This question yielded an average response of 3.00/5, suggesting a neutral stance regarding students use of the software in future classes. As this is a senior design course, students are less likely to take future classes, which explains the lower average.

Students were then asked the same question with respect to their future careers. Figure 5 shows an average response to this question of 2.86/5, suggesting that students slightly disagreed with the statement that they would use Polymer Genome in their professional career. Collectively, these findings suggest that students appreciate the industrial potential of Polymer Genome (Figure 3) but potentially view it as more useful in the classroom, given that its application in industry is closely tied to students future involvement with polymer systems.

Overall the responses in Figures 4 and 5 appear to be influenced by students education and career paths. Figure 3 indicates that the instructional lectures successfully conveyed the industrial relevance and practical applications of Polymer Genome.

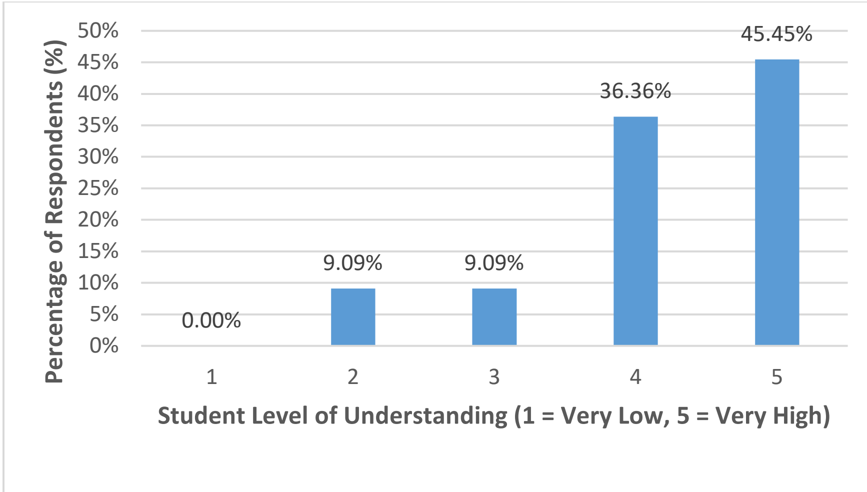

Figure 3. Survey Results Showing Students Understanding of How Polymer Genome Could Be Applied in Industry (avg = 4.18/5, n = 22)

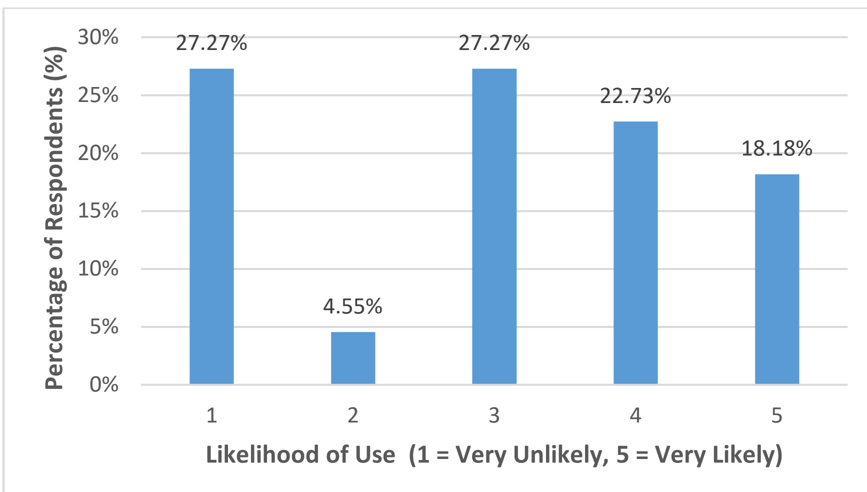

Figure 4. Survey Results Showing Students Ratings of How Likely They Were to use Polymer Genome in Their Future Classes (avg = 3.00/5, n = 22)

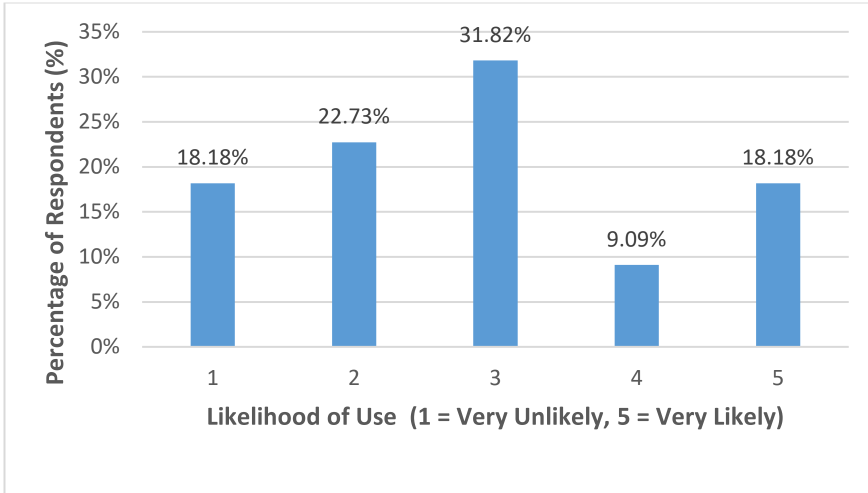

Figure 5. Survey Results Showing Students' Ratings of How Likely They Were to use Polymer Genome in Their Future Careers (average = 2.86/5, n = 22)

Section 2: PolyBERT

To maintain consistency, the questions in this section followed the same format as those in Section 1, allowing for direct comparison of students' understanding of the two software tools. Students first were asked to rate their understanding of how PolyBERT works and how it estimates polymer properties. Figure 6 shows an average response of 3.64/5, establishing that students had a very similar level of understanding of the methodologies used by PolyBERT and Polymer Genome. Similar to Polymer Genome, it is possible that students who rated their understanding of PolyBERT as a 1 or 2 did so primarily due to limited prior exposure to AI-based engineering tools.

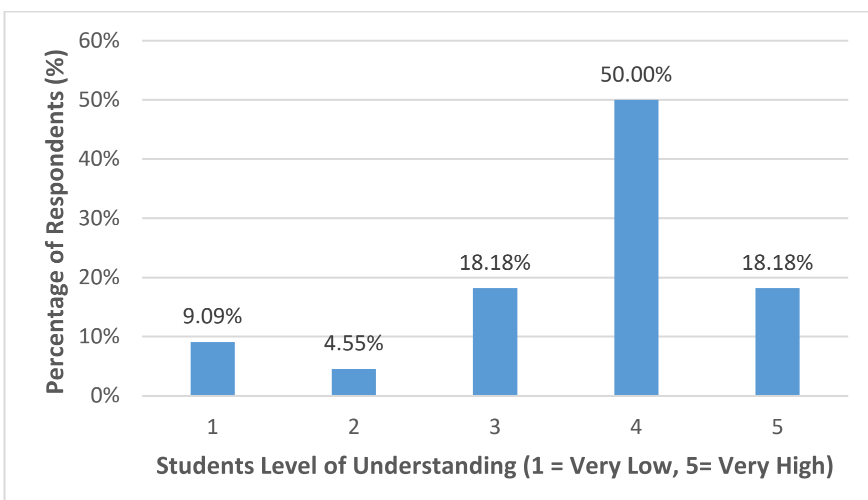

Figure 6. Survey Results Showing Student Understanding of PolyBERT after Instructional Lectures (average = 3.64/5, n = 22).

Next, the students were asked to assess their understanding of the advantages and disadvantages of PolyBERT, with the results shown in Figure 7. This question received an average rating of 3.95/5, indicating a strong overall level of comprehension of PolyBERTs advantages and disadvantages.

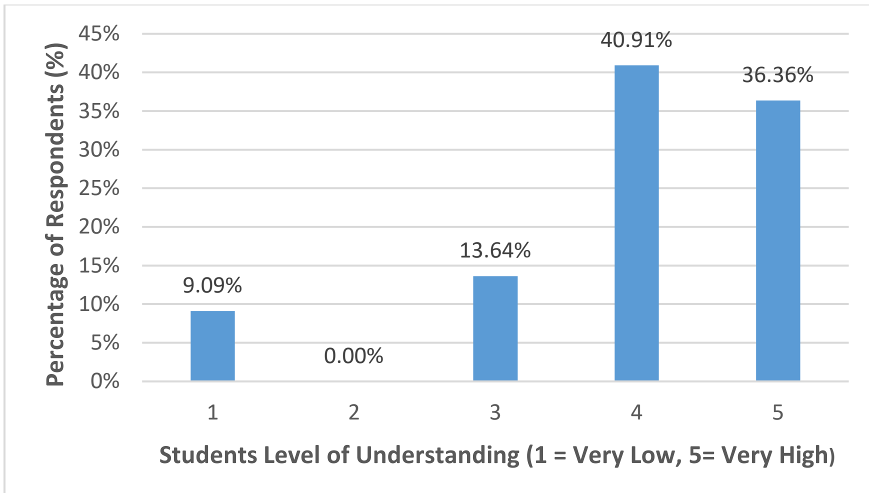

Figure 7. Survey Results Showing Students Understanding of the Advantages and Disadvantages of PolyBERT (average = 3.95/5, n = 22).

Students were asked to assess their understanding of how PolyBERT could be applied in industrial settings, yielding an average rating of 4.09/5, as shown in Figure 8. Although slightly lower than the corresponding rating for Polymer Genome, this result indicates that students were able to recognize PolyBERT's potential industrial applications. Figures 9 and 10 demonstrate that when students were asked how likely they were to use PolyBERT in future coursework and careers, they reported average ratings of 2.86/5 and 2.82/5, respectively. These values were slightly lower than those reported for Polymer Genome, suggesting that while students understood PolyBERT's applicability in industry, they were less inclined to use the software personally and potentially preferred Polymer Genome. This trend can likely be attributed to Polymer Genome being faster and easier to use compared to PolyBERT, making it more advantageous in an industry setting.

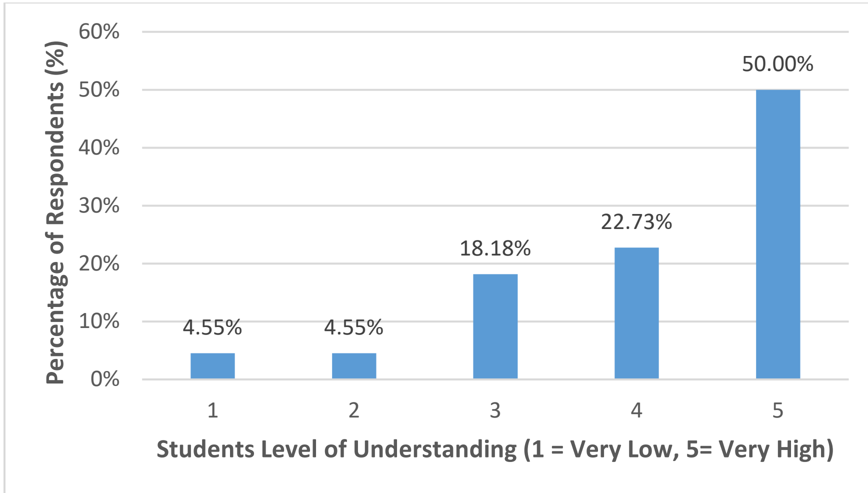

Figure 8. Survey Results Showing Students Understanding of How PolyBERT Could be Applied in Industry (avg = 4.09/5, n = 22).

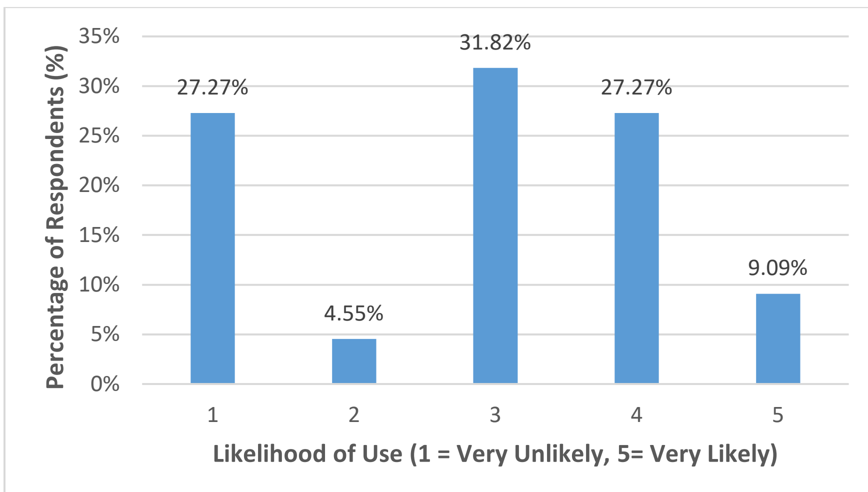

Figure 9. Survey Results Showing Students' Ratings of How Likely They Were to use PolyBERT in Future Classes (average = 2.86/5, n = 22).

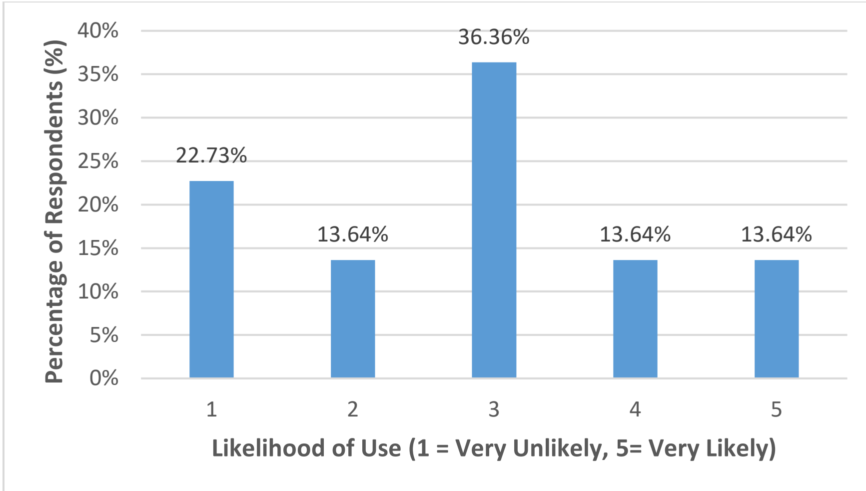

Figure 10. Survey Results Showing Students' Ratings of How Likely They Were to use Polymer Genome in Their Future Careers (average = 2.86/5, n = 22)

Section 3: Feedback on Lectures and Project

Following their evaluation of the two software tools, the students were asked to reflect on the project and lectures in the form of student comments. As is shown in the example comments below, the student feedback was positive, suggesting that the project and lectures effectively enhanced both their understanding of AI concepts and their ability to use Polymer Genome and PolyBERT.

> *Yes! Doing the short project made me understand the difference between AI and machine learning which I did not understand before.*

> *Yes, I feel that the polymer project was extremely helpful in enhancing my understanding of AI and machine learning. Beyond AI tools like Meta or ChatGPT, I did not know of the many applications for AI, specifically in engineering. I had zero knowledge of ML prior to this assignment, and I now feel I have a basic understanding of the subject.*

> *I felt that the short polymer project enhanced my understanding of polymer genome and polyBERT because it allowed me to gain hands-on experience with both platforms. By working with both models, I was able to somewhat grasp their complexities.*

Students were asked whether they believed Polymer Genome and PolyBERT would be useful to them in the future. While a majority of students indicated that the tools could be beneficial, many noted that their usefulness would be highly dependent on their specific career paths.

> *They could depending on what career I decide to continue with. As of right now it's not something that's really needed for water treatment.*

> *I feel like these two tools could be useful in the future if I pursue a career that involves the use of polymer estimation. I do not think I will have such career, but if I did I could see how this is extremely useful.*

I feel like these tools would be very useful for me if I end up in R&D. These open up to new polymer properties, which perfect for research applications. I can see myself using the tools for production as well but not so much.Section 4: Students Perception of AI Integration

Students were asked whether AI and machine learning should be implemented in future engineering classes. The responses reflected generally positive perceptions of integrating AI into engineering coursework. Several students noted that exposure to these AI tools would benefit them in preparing for the industry. There were no significant concerns raised about the environmental impacts of AI. However, some students emphasized the importance of teaching ethical considerations related to AI and maintaining a level of skepticism regarding its conclusions on various subjects. Some students' comments can be seen below.

I think implementing AI and machine learning is beneficial in the future because the world is becoming increasingly more dependent on technology and this is another platform that will likely be heavily used in the future as advancements are made.

I think it is so important because it is so prevalent today and understanding more than just ChatGPT could help to stand out in interviews.

I think implementing AI and machine learning in classes in the future could definitely be beneficial if used correctly, because the computing capabilities would make many things much easier than before. The ability to consult AI or machine learning programs also has the ability to potentially save time when looking for certain information or solving certain types of problems.

Conclusions and Future Work

Using the survey results and feedback from students, the lectures and associated project will be refined for future classes. One major theme in the student feedback was the desire for additional lecture time to allow for a slower pace and improved digestion of the material. Students also reported difficulty with the fundamentals of Python coding, which is not currently taught in the undergraduate program. To address this, a dedicated lecture will be added to focus specifically on Python programming skills as they relate to the project. Another commonly cited suggestion was the inclusion of more in-class examples demonstrating the use of PolyBERT code. Adding this to future lectures could improve student engagement and comprehension. These lectures and the associated project could also be incorporated into other chemical engineering courses, such as computer methods, separations, and polymer processing, to further support student learning by providing repeated exposure to the material.

In future offerings of the class, a pre-course survey will be conducted to assess students' familiarity with generic AI large language models as well as engineering-specific AI tools. This initial assessment will help inform targeted instructional design and allow for a quantitative comparison of students' perceptions, confidence levels, and tool competency before and after the course. Additionally, in future offerings, it would be beneficial to implement structured discussions on ethical considerations and environmental impacts of large language models, as well as the responsible use of AI in engineering design. From this, questions assessing students' support and ethical concerns related to AI tools can be analyzed.

Although project type was not recorded in this study, the majority of students did not have polymer focused capstone projects, however overall ratings for Polymer Genome and PolyBERT were largely positive. This suggests that perceived value of AI based engineering tools may be largely independent of the students project type. Future work should examine how project alignment influences student perception and adoption of such tools.

Overall, integrating these lectures and projects into a chemical engineering capstone design course was beneficial to students and helped better prepare them for future engineering careers. The project, which incorporated Polymer Genome and PolyBERT, enhanced the learning experience by introducing students to AI-driven tools and expanding their engineering skill sets. Based on survey responses, the students generally preferred Polymer Genome over PolyBERT, likely due to its ease of use and accessibility. Nonetheless, the survey results indicated that students viewed the experience positively and recognized the value of gaining exposure to AI applications in engineering, particularly given the growing role of AI in industrial practice. Given these positive outcomes, further expansion of lectures addressing both general AI concepts and engineering-specific AI applications may be beneficial in future courses.

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