

INNOVATIVE USE OF ARTIFICIAL INTELLIGENCE IN A MATERIALS SCIENCE SUBJECT FOR ANALYZING RESULTS

Jaume Gomez-Caturla, Lourdes Sanchez-Nacher, Teodomiro Boronat, Octavio Fenollar, Carlos Lazaro-Hdez, & Rafael Balart

Universitat Politècnica de València, Dpto. de Ingeniería Mecánica y de Materiales, Escuela Politécnica Superior de Alcoy (Spain)

Abstract

Artificial intelligence (AI) is gaining increasing interest over the years, and it is one of the most useful tools to be used in education, either in primary and secondary education or in university. AI is a very powerful tool to show students how to be more independent and make them main characters of their own learning. In this study, AI is used in a subject called Structures and Characterization Techniques from the masters' degree Engineering, Processing and Characterization of Materials from Universitat Politècnica de València (UPV). The main aim of this study is using AI models, such as ChatGPT or DeepSeek to help students analyse results obtained in the aforementioned subject. In this subject, different polymeric materials are characterized and their properties are evaluated. However, some properties, such as chemical bonds present in those materials are normally quite difficult to evaluate and understand by students. These chemical bonds are characterized by Fourier Transformed Infrared Spectroscopy (FTIR), which gives a spectra with different peaks associated with the chemical interactions in the molecules of the analyzed materials. The students use AI models for assisting them in analyzing these FTIR spectra. Moreover, the analysis made by students is compared with a traditional FTIR analysis. Results show that, in general, the effectiveness of AI models is superior and easier for students to use. This is corroborated by surveys made to students at the end of the subject.

Keywords: *AI models, FTIR, characterization, materials.*

1. Introduction

Artificial Intelligence (AI) is increasingly being recognized as a transformative force in education, offering novel ways to engage students, personalize learning, and improve educational outcomes across all levels—from primary to higher education. In university settings in particular, AI is not only enhancing pedagogical practices but also enabling students to take a more active and independent role in their learning processes. The use of AI in this context aligns well with the evolving educational paradigm that values critical thinking, autonomy, and the ability to engage with complex, interdisciplinary problems (White, 2020).

One of the most promising applications of AI in higher education lies in its ability to support students in analyzing and interpreting complex data (Pierdicca and Paolanti, 2022). This is particularly relevant in scientific and technical disciplines where understanding nuanced experimental results is a critical skill. In the master's program Engineering, Processing and Characterization of Materials at Universitat Politècnica de València (UPV), AI models such as ChatGPT and DeepSeek have been integrated into the curriculum of the subject Structures and Characterization Techniques. Here, AI is used as a pedagogical aid to assist students in interpreting experimental data—specifically the characterization of polymeric materials through techniques like Fourier Transform Infrared Spectroscopy (FTIR).

FTIR spectroscopy is a common method for identifying chemical bonds in polymeric materials by analyzing the peaks in the infrared spectrum (Ismail et al., 1997). However, understanding and interpreting these spectra can be particularly challenging for students due to the complexity of chemical interactions and the subtle differences in peak patterns. By incorporating AI tools into the learning process, students are given the ability to receive real-time assistance in analyzing FTIR data and understanding the molecular structures of the materials they study. This use of AI transforms what can often be an abstract and difficult subject into a more accessible and interactive learning experience.

Notably, the AI-supported approach is not meant to replace traditional methods but to complement and enhance them. In the UPV case study, students are meant to obtain FTIR spectra from two different polymers, high density polyethylene (HDPE) and polylactic acid (PLA), analyze both spectra by the traditional methodology and by AI-supported methodology, and are encouraged to compare their AI-assisted analyses with traditional FTIR interpretation techniques based on literature. In addition, feedback is collected from the students through surveys, relating to the comfortability of obtaining complex data using AI databases, in this case ChatGPT.

This study is meant to underscore the growing potential of AI to support higher education, particularly in technical disciplines where data interpretation plays a central role. As AI tools become more sophisticated and accessible, their integration into university curricula can foster deeper engagement, independent learning, and improved academic performance. However, successful implementation also requires thoughtful integration, faculty training, and an emphasis on ethical and critical use of these technologies.

2. Objectives

The objective of this study is to explore the effectiveness of integrating artificial intelligence tools, specifically ChatGPT and DeepSeek, into the Structures and Characterization Techniques course within the master's degree in Engineering, Processing and Characterization of Materials at Universitat Politècnica de València. The focus is on evaluating how these AI models support students in interpreting complex data, particularly Fourier Transform Infrared Spectroscopy (FTIR) spectra used to characterize polymeric materials. By comparing AI-assisted analyses with traditional methods and gathering student feedback, the study aims to assess the impact of AI on learning outcomes, student autonomy, and overall engagement.

3. Methods

In this study, a class of 15 students in the subject of Structures and Characterization Techniques in the master's degree in Engineering, Processing and Characterization of Materials was taken as a sample. One of the aspects of the work in this subject is analyzing the FTIR spectra of several polymers, in this case: high density polyethylene (HDPE) and polylactic acid (PLA). The analysis is carried out using a Bruker S.A Vector 22 (Madrid, Spain) coupled to a PIKE MIRacle single reflection diamond ATR accessory (Madison, Wisconsin, USA). 20 scans were taken and averaged for each measurement, between 4000 and 600 cm^{-1} . Once the spectra of both polymers was obtained, students were asked to evaluate them using IA models (ChatGPT or DeepSeek) and searching in scientific literature. Afterwards, surveys were conducted in order to assess the comfortability of students towards this new approach to evaluate more abstract and complex data such as FTIR spectra.

4. Discussion

4.1. FTIR analysis

The main scientific data obtained by students in this study was that of FTIR spectra from HDPE and PLA polymers. Figure 1 shows the spectra of both polymers made by the students. FTIR is one of the most difficult characterization techniques for students to evaluate and comprehend. Moreover, the traditional approach of analyzing it through literature is rather time consuming and not the most attractive activity for students, as it will be discussed in the following section.

Table 1 gathers an FTIR analysis made by a student of both spectra presented in Figure 1. This analysis has been done with and without the help of AI models. As it can be observed, the AI analysis fully comprehends all the wavenumber range taken in the spectra, selecting the most important peaks and bands and associating them to the corresponding chemical bond present in the polymer. Moreover, it gives certain details that add more accuracy to the evaluation and help to better understand the nature of the polymer. On the other hand, the analysis done without AI models was correct up to a point, but was missing some important details and some of the most important bands in the spectra.

Figure 1. FTIR spectra of high density polyethylene (HDPE) and polylactic acid (PLA).

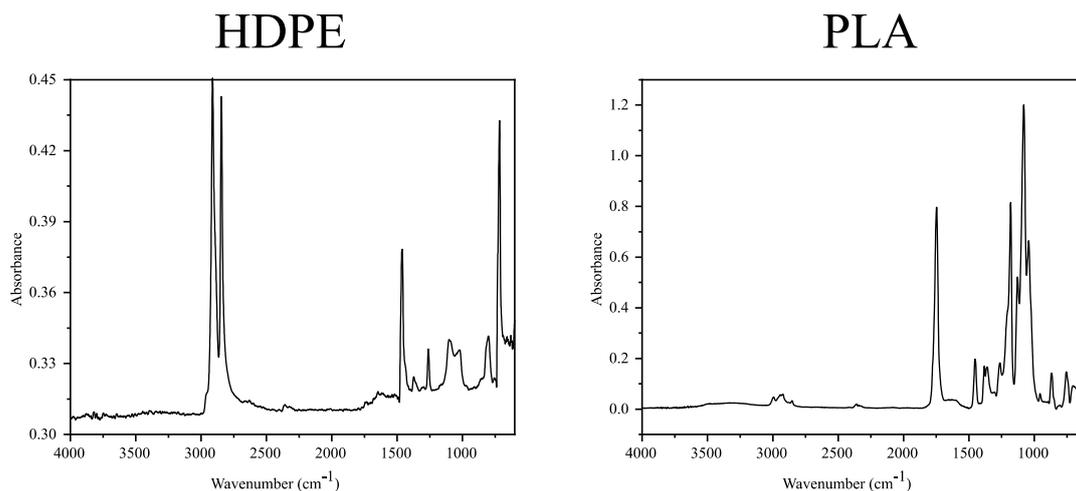


Table 1. Evaluation of the FTIR spectra made by a student based on ChatGPT AI model.

Wavenumber (cm ⁻¹)	HDPE functional groups (AI analysis)	HDPE functional groups (traditional analysis)	Wavenumber (cm ⁻¹)	PLA functional groups (AI analysis)	PLA functional groups (traditional analysis)
2950	Asymmetric CH ₂ stretching	CH ₂ – asymmetric stretching	2995-2945	C-H stretching (weak to moderate signaling corresponding to methyl and methine stretches.	C-H stretching
2915	Asymmetric CH ₂ stretching	CH ₂ – asymmetric stretching	1750	Strong C=O stretching. Signature peak of the ester group in PLA	C=O stretching
1472	CH ₂ bending		1455	CH ₃ bending (deformation)	CH ₃ bending
1462	CH ₃ bending	CH ₃ bending	1360	CH bending	CH bending
1375	CH ₃ symmetric bending	-	1180-1080	C-O-C stretching. Presence of multiple strong peaks that indicate symmetric and asymmetric stretching of the typical ester linkage of PLA.	C-O-C stretching
730 - 720	Rocking vibration of (CH ₂) _n sequences – particular characteristic of long alkyl chains, typical of PE	Rocking vibration of -CH ₂ -	870-750	C-COO out of plane bending. Less intensity but it can appear depending on the crystallinity and structure of PLA.	-

4.2. Students' feedback

In the final session of the subject, a satisfaction survey was conducted in all students in order to receive feedback from them about the use of AI. This was very interesting for us, as FTIR is a complex technique that every year gives rise a lot of doubts and misunderstandings about how to analyze the obtained results and how to interpret them. Table 2 shows the answers to 10 questions to which the students responded yes, no or left it blank. In general, it can be seen that the feedback was positive, as it was expected. It was observed that students found it a lot easier to analyze FTIR by using ChatGPT or DeepSeek than by the traditional method of consulting literature. Moreover, it was less time consuming and as described by some students, not so “boring”. In addition, we knew that after making the analysis of the

FTIR spectra as it was required, some student further investigated about the polymers they had just analyzed, searching for their origin, applications and looking for more details about their chemical structure. This survey reflects that the use of AI is perfect for making it easier and more constructive for students to analyze complex data in the laboratory, and that it even motivates them to investigate further than what it was required.

Table 2. Answers of the students to the satisfaction survey conducted at the end of the subject.

Question	Number of students that answered		
	Yes	No	Blank
1. Have you ever received AI teaching methodologies in any other subject before?	1	14	0
2. Would you include AI teaching in other subjects?	13	2	0
3. Would you maintain this methodology for the next year?	13	1	1
4. Have you enjoyed using AI more than consulting literature?	10	3	2
5. Do you consider it has been easier to analyze FTIR by AI than by consulting literature?	14	0	1
6. Do you consider that your results have been better due to the use of AI models?	15	0	0
7. Do you think that the results obtained through literature have been more complete than by AI?	0	15	0
8. When you conducted the FTIR analysis by AI, did you find it more time consuming than the traditional analysis?	1	14	0
9. Did you explore further about the FTIR analysis than what it was initially required in the subject through AI?	9	3	3
10. Are you satisfied with the AI methodology used in the laboratory practices of the subject?	14	0	0

5. Conclusions

This work has proven that AI methodologies can be effectively used in practical laboratory sessions of Materials based subjects. In spite of the fact that the approach taken in this study is simple, it has considerably improved both the results of the students and their attitude towards the subject and the FTIR technique. In previous years, FTIR was seen as very complex and abstract by students, which made them dislike this part of the subject. However, this year, the use of AI has improved the concern of the students for this technique, has made them better understand it, and has also encouraged them to further investigate about the insights of FTIR and the results it provides. It has also been demonstrated the potential of AI for analyzing complex data with more ease, which can also be transferred to other different complex methodologies and even in other subjects. We plan on developing more complex approaches using AI in future years both in this subject and in other materials-based subjects.

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