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Article

Advancing Life Cycle Assessment of Sustainable Green Hydrogen Production Using Domain-Specific Fine-Tuning by Large Language Models Augmentation

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Abstract: Assessing the sustainable development of green hydrogen and assessing its potential environmental impacts using the Life Cycle Assessment is crucial. Challenges in LCA, like missing environmental data, are often addressed using machine learning, such as artificial neural networks. However, to find an ML solution, researchers need to read extensive literature or consult experts. This research demonstrates how customised LLMs, trained with domain-specific papers, can help researchers overcome these challenges. By starting small by consolidating papers focused on the LCA of proton exchange membrane water electrolysis, which produces green hydrogen, and ML applications in LCA. These papers are uploaded to OpenAI to create the LlamaIndex, enabling future queries. Using the LangChain framework, researchers query the customised model (GPT-3.5-turbo), receiving tailored responses. The results demonstrate that customised LLMs can assist researchers in providing suitable ML solutions to address data inaccuracies and gaps. The ability to quickly query an LLM and receive an integrated response across relevant sources presents an improvement over manually retrieving and reading individual papers. This shows that leveraging fine-tuned LLMs can empower researchers to conduct LCAs more efficiently and effectively.

Keywords: life cycle assessment; green hydrogen; machine learning; customised large language model

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1. Introduction

Green hydrogen is crucial for the future of renewable energy [1], and water electrolysis for hydrogen production is used to produce green hydrogen by utilising electricity generated from renewable energy sources [2]. Currently, the primary mature technologies for water electrolysis include Proton Exchange Membrane Water Electrolysis (PEMWE), Alkaline Water Electrolysis (AWE) and Solid Oxide Electrolysis Cells (SOEC) [2]. PEMWE boasts higher hydrogen production efficiency compared to AWE [3], while SOEC is not yet feasible for large-scale commercialisation [4]. Compared to AWE and SOEC, PEMWE offers greater adaptability to renewable energy sources [3] and is considered the most promising technology in terms of sustainability and environmental impact [4]. To measure the environmental impact of PEMWE in green hydrogen production, it is essential to assess its life cycle using the Life Cycle Assessment (LCA) approach. The LCA will comprehensively analyse the potential environmental impacts of PEMWE to optimise its application and improve overall sustainability [5,6].

However, conducting an LCA faces challenges, particularly related to data issues such as inaccuracies and missing environmental data [7]. Machine learning (ML) has emerged as a promising solution to address these challenges. Many studies have shown that it can effectively help solve the data-related challenges in LCA, such as using artificial neural networks (ANNs) to estimate the missing data or predict potential future environmental impacts, thereby improving the accuracy and reliability of LCA [7]. However, finding these ML methods typically requires a significant time investment in reviewing the literature or consulting experts. Therefore, in this paper, the idea of using customised large language models (LLMs) to help find suitable ML solutions to address LCA challenges is presented.

Large Language Models (LLMs) have emerged as cutting-edge artificial intelligence systems that can process and generate text with coherent communication [8], and generalise to multiple tasks [9–11]. Although pre-trained LLMs have excellent generalisation capabilities, they must be fine-tuned to follow specific instructions and generate safe responses [12] for effective utilisation. Contextual augmentation helps LLMs to learn from the examples of concatenated inputs. This enables the LLMs to answer specific queries beyond the capacity acquired during training by producing factually correct and safe responses [9]. Studies such as [13,14] explore the strengths, weaknesses, risks and opportunities associated with leveraging LLMs to support LCA practitioners. These studies also evaluate the capability of generalised LLMs to perform various LCA tasks. Their findings suggest that LLMs have considerable potential to enhance the development of life cycle inventories and to effectively summarise and communicate LCA results. This, in turn, could lead to improved LCA quality while significantly reducing the time required to complete an assessment. LLMs are used in this study as they show significant potential for providing qualitative and quick research, which allows optimisation of time and resources spent in the drafting stage of an idea [15]. In this study, the LLM models were trained with research papers related to the LCA of PEMWE and the application of ML in LCA. When researchers query the customised LLM, the responses are tailored to specific queries. The results indicate that the customised LLMs significantly assist researchers in producing valuable outcomes by identifying appropriate ML solutions to address data inaccuracies and gaps. This underscores how leveraging LLMs empowers researchers to conduct LCAs more efficiently and effectively.

The Section 2 of the paper provides a brief theoretical background on LCA, PEMWE, and issues encountered in conducting LCA for PEMWE and LLMs. Section 3 extensively explains the methods used in the study, including the fine-tuning strategy of LLMs and prompt generation techniques. Section 4 presents the results and discussion of the customised LLMs' responses to five example questions. The Section 5 summarises all findings, highlighting how LLMs can significantly assist researchers in managing the complexities of LCA by offering qualitative insights and suggesting appropriate ML approaches to address data inaccuracies and deficiencies. The strengths and weaknesses of the customised LLMs are summarised along with a discussion of the approaches which are required to improve the results in the future.

2. Background

2.1. Life Cycle Assessment

LCA is a comprehensive methodology that evaluates the environmental impacts of all stages of a product's life cycle, from raw material extraction to production, use and disposal. The four phases for conducting an LCA as outlined by ISO 14040 and ISO 14044 are as follows [5,6]:

1. Goal and Scope Definition: Defining the assessment's purpose, scope and boundaries.
2. Life Cycle Inventory (LCI): Collecting data on the inputs and calculating the potential environmental outputs of the product system, collecting input data and calculating the product system's potential environmental outputs.
3. Life Cycle Impact Assessment (LCIA): Categorising and evaluating potential environmental impacts based on the LCI results.
4. Interpretation: Analysing results to make informed decisions.

2.2. General LCA Challenges and Application of ML Techniques

In this section, examples are used to showcase the challenges that exist in LCA studies and provide methods using ML that have been employed to address these challenges.

- Data Gaps: Environmental results generated from LCI databases frequently exhibit inconsistencies or gaps in data availability [7]. For example, Kalverkamp et al. [16] presented the issue of lacking suitable environmental data for different regions. Their case study showed that the ecoinvent database had limitations in providing environmental data for raw materials manufactured in China [16]. In this context, the only China-specific data used are for "electricity, medium voltage, at grid", "lithium hexafluorophosphate, at plant" and "ethylene carbonate, at plant" [16]. For other components and processes relevant to China, they had to rely on global average data provided by ecoinvent [16]. This data gap underscores the challenges in conducting accurate lifecycle assessments with incomplete regional. Furthermore, existing datasets often contain outdated information and require updates to reflect current practises, such as adjusting input data for solar panels based on the electricity source [17].
  To address these challenges, according to the literature review from Romeiko et al. [7], several studies about LCA have utilised approaches such as linear regression models, artificial neural networks (ANN) and random forest algorithms to predict or estimate environmental emissions, such as greenhouse gas emissions or the release of organic chemicals during the operational phase [7]. Additionally, these approaches are used to predict missing product characteristics, for example, forecasting biobased chemicals derived from hydrothermal treatment [7].
- Uncertainty: Variability in data sources and methods can introduce significant uncertainty into the LCA results. As summarised in Romeiko et al., challenges in interpreting LCA results include identifying where the highest impact lies (identifying hotspots), which involves conducting uncertainty and sensitivity analysis [7]. Questions arise regarding why these hotspots occur, what factors contribute to them and how they can be mitigated. ML approaches such as ANN, ANFIS, BRT, random forest, genetic algorithms, centroid-based clustering and logistic regression can be utilised for analysing the uncertainty and sensitivity of LCA results [7].

These examples only illustrate some of the challenges that arise in LCA and their corresponding ML solutions. In addition to these challenges, there are other issues in LCA, such as how to select LCI databases and LCIA methods.

The variability in environmental outcomes across different LCI databases poses a challenge in determining which database to prioritise, such as choosing between ecoinvent [18] and Sphera database (formerly known as the GaBi database) [19,20]. The reasons for making a choice include, as highlighted by Pauer et al. [19], that in many cases, the ecoinvent contains considerably more background processes (e.g., wear and tear of infrastructure, maintenance work, etc.) than Sphera [19]. For example, the generation of 1 kWh of electricity from nuclear energy in Germany shows that the result for "ionising radiation" in ecoinvent is twice as high as in Sphera [19]. This higher value in ecoinvent is mainly due to the dumping of overburden from uranium ore mining [19]. Furthermore, choosing between different databases also involves considering their data transparency and the flexibility to tailor the data according to users' requirements [21].

The variability in results can also be derived from different LCIA methods [19,22–24]. LCIA can be conducted at two assessment levels: midpoint and endpoint [25]. Different LCIA methods categorise LCI results differently, for example, ReCiPe 2016 normalised the characterisation factors (LCI results) into different midpoint environmental categories [26]. Normalisation allows users to see the relative contribution of each impact category to the overall system, which is particularly useful when addressing specific regional environmental challenges [25]. At the endpoint level assessments can be normalised or weighted, and only the EF v3.0 method can obtain weighted results at the midpoint level and the endpoint level and combine them into a single score [27]. For example, in the study by Domingo-Morcillo et al. [25] on the LCA of food loss and waste prevention and reduction, they aimed to clarify which impact categories are more significant through weighting, making it suitable for comparing and selecting the "best option", thereby providing a comprehensive basis for decision-making [25]. However, for non-LCA professionals, distinguishing between each LCIA method and selecting the most appropriate one based on their needs can be a challenging task.

2.3. LCA for PEMWE and Its Challenges

In this section, the different phases of LCA for PEMWE are introduced and the corresponding challenges identified are described. The life of a PEMWE can be divided into three main phases: construction, operation and end of life [28,29]. During the construction phase, the entire PEMWE plant will be built [28]. In the operation phase, the plant will produce hydrogen from electricity and water [28]. The end-of-life phase occurs when the plant reaches the end of its lifespan and faces either disposal or recycling [28]. To understand the potential environmental impact of the entire life cycle of a PEMWE plant, its LCA can be conducted in four phases according to ISO 14040 and 14044 [5,6].

Phase 1: This phase involves defining the system boundaries and the purpose of conducting the LCA. This includes specifying where the PEMWE plant is analysed (geographical boundary), the operational lifespan of PEMWE (time boundary), etc. [5,6]. Additionally, define the functional unit, which serves as a basis for all data collection, calculation and presentation of results [5,6,28].
Phase 2: The second phase is the LCI, where all the technical data of PEMWE are collected, such as the material inputs in the construction phase, energy demand in the operational phase, etc., and the life of PEMWE will be modelled using software (e.g., Umberto [30], Brightway [31] etc.) to generate LCI results showing various potential environmental results.
Phase 3: The third phase is LCIA, also conducted using software. Here, environmental results from the second phase, LCI, are categorised and summarised into different impact categories, such as human toxicity, resources, climate change, etc. [5,6]. Different LCIA methods categorise results differently, each using its distinct approach, such as ReCiPe, EF [32], etc. [33]
Phase 4: The final phase is interpretation, where the LCIA results are analysed. This includes conducting sensitivity analysis to understand the reasons behind PEMWE's varying environmental impacts at different life phases [5,6]. With this understanding, informed recommendations can be made to promote the more environmentally friendly development of PEMWE.

The primary challenge identified in current LCA studies on PEMWE lies in missing or inaccurate technical input data. For example, there is a notable absence of recycling potential data (e.g., recycling rate of specific material) in the end-of-life phase of PEMWE [28]. Additionally, there are data gaps for specific components in the Balance of Plant (BOP), such as technical specifications for hydrogen purification [28,34]. Moreover, in many cases, secondary data sources (e.g., data from literature) are predominantly used due to the limited availability of primary data (e.g., experimental data), particularly concerning renewable energy-based electrolytic technologies [35].

2.4. Large Language Models (LLMs)

An LLM is an advanced machine-learning model based on the transformer architecture. The transformer architecture was first proposed in the research paper "Attention is All You Need" [36]. The self-attention mechanism of this transformer architecture allows the models to weigh the significance of different words in a sentence, irrespective of their relative position. This feature enables the model to capture complex syntactic and semantic dependencies more effectively than previous architectures [37]. An LLM, like OpenAI's GPT (Generative pre-trained transformer) series, is specifically designed and trained for natural language processing tasks. These models contain tens to hundreds of billions of parameters pre-trained on vast amounts of text data and can generate human-like text, understand context, and answer questions. Examples of LLMs include BERT [38], RoBERTa [39], GPT-3, GPT-4 [40] and LLaMA [41]. The advanced capabilities of these models include (1) contextual learning, where LLMs can grasp and learn from a few examples provided during inference; (2) following instructions, where after being tuned with instructions, LLMs can perform new tasks based on guidelines without needing explicit examples; and (3) multistep reasoning, where LLMs solve intricate problems by breaking them down into intermediate reasoning steps, as seen in chain-of-thought prompting. In this framework, LLMs can aid engineers in conducting life cycle assessments by supplying domain-specific knowledge in natural language [42]. LLMs have demonstrated significant potential in scientific research, with applications ranging from literature review and code development to modelling complex biological sequences and parsing qualitative data [43]. In the medical domain, LLMs show promise in enhancing the quality and efficiency of research and scientific writing [44]. LLMs have been applied to textual knowledge, small molecules, macromolecular proteins and genomic sequences in the biological and chemical domains, focusing on model architectures, capabilities, datasets and evaluation [45]. LLMs such as ChatGPT, Gemini 1.5 and Claude 3.5 are designed to generate human-like text by analysing vast datasets of text data [46]. These models use deep learning techniques to understand and predict text patterns, making them capable of producing coherent and contextually relevant content. They have shown remarkable abilities in various tasks, including predicting electromagnetic spectra [47] and automating text analytics and generation [48]. However, they also pose significant challenges and risks, including perpetuating biases and the exclusion of non-majority languages [48]. The potential of LLMs to revolutionise research is significant, but their use must be transparent and ethical [15].

Most notably, LLMs can contribute to idea generation and drafting sections of research papers. However, their limitations in providing accurate citations and identifying genuine research gaps necessitate human oversight [49]. The integration of LLMs into scientific research offers both opportunities and challenges. LLMs can boost productivity and foster innovation by streamlining literature reviews, enhancing scientific writing and modelling complex biological sequences [43]. Researchers and peer reviewers require guidelines and norms to ensure their ethical application, especially regarding AI-generated content [50]. This study aims to help researchers find appropriate ML solutions to address their LCA challenges more effectively, utilising the capabilities of LLMs to achieve this goal. After gaining a particular understanding of the use of ML in LCA and the application of LLMs in the research field, in the next section, the progress of training the LLMs to find ML solutions for LCA challenges related to PEMWE is outlined.

3. Methodology

This section details a specific approach to using customised LLMs to discover ML solutions for LCA challenges. A visual representation of the methodology used in the paper is shown in Figure 1. The graphic shows the "classic human strategy" is based on reviewing papers with the help of human intelligence to find the solutions for the challenges of LCA for PEMWE. Furthermore, another strategy is the "classic LLM strategy", in which the questions of challenges are to directly query a pre-trained stock LLM to provide suitable responses to the challenges of the LCA without referring directly to papers related to the topic. A more effective approach is combining these two strategies into a fine-tuned, customised LLM trained with relevant scientific research papers. This tailored approach enables the LLM to provide more accurate and context-specific answers to the challenges. Further details of this approach are discussed in the following sections.

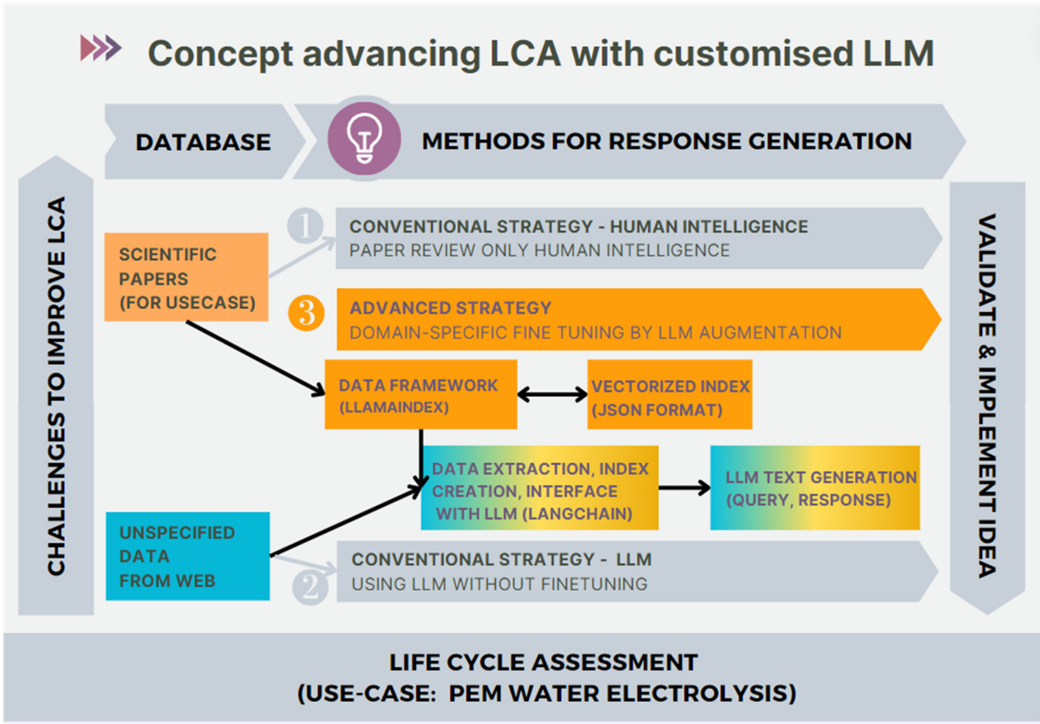

Figure 1. Concept advancing LCA with customised LLM. When challenges arise in LCA, in addition to using human intelligence (HI) by reading scientific papers (path 1) and employing non-finetuned LLMs (path 2) to find solutions and methods, path 3 is offered, where LLMs are fine-tuned and trained to address ideas of solutions for challenges that be encountered in the LCA of PEMWE. The fine-tuning process involves storing the relevant scientific papers into a data framework. These papers are vectorised using LlamaIndex within the LLMs, then integrated with other unspecified online resources (LangChain), providing LLMs with a broad information base to generate a customised response.

3.1. Fine-Tuning Strategy of LLM with Augmentation Techniques

The pre-trained LLMs can be used to generate desired outputs for various tasks. However, to exploit the full potential or to address their shortcomings, such as hallucinations, the augmentation of the models by providing domain-specific knowledge externally is needed [42]. In this contribution, stock LLMs are combined with the retrieval-augmented generation (RAG) approach to steer them towards more factual outputs. RAG is a methodology that integrates external data sources during inference, allowing the model to retrieve relevant information and generate more accurate responses. This approach simplifies data management and helps mitigate the inherent probabilistic nature of LLMs.

Another primary limitation of the stock pre-trained LLMs is their lack of up-to-date knowledge or access to private or use-case-specific information. Therefore, integrating an external database to the LLM to retrieve relevant information from the reference databank enables the model to generate a context-specific customised response to the questions. As mentioned earlier, OpenAI built the GPT LLM model series, including GPT-3 and GPT-4. ChatGPT is a web-based chatbot application that leverages the powerful GPT-3 model to facilitate fine-tuned optimal dialogue interactions. OpenAI also offers a feature for creating customised GPTs to harness the power of the LLMs using a custom dataset for augmentation. Subsequently, this customised GPT LLM is used in this work and can respond to inquiries based on the content within these research papers. The GPT models can be augmented with relevant research related to PEMWE and ML applications for LCA using this feature. The model retrieves specific documents from the curated corpus using LlamaIndex and LangChain and integrates these data into the LLM's output during inference, which is consistent with the RAG approach. OpenAI's customised GPT model is based on components such as LlamaIndex and LangChain, which provide a framework for interacting external data with LLMs. LlamaIndex is a data framework that provides a simple, flexible interface to connect the LLMs with external data. It creates a vectorised index of the document data to enable efficient queries. LangChain provides an application programming interface to access and interact with LLM and facilitate seamless integration for various use cases. The combination of the Llamaindex and LangChain provides the framework to augment context-specific GPT models with customised datasets and further develop applications. This approach is visually represented in Figure 1. The current approach consolidates the research papers that train the custom GPT model into a single folder. These files are uploaded into the OpenAI interface, forming the basis for constructing the LlamaIndex. These data are then vectorised, and the resulting index is saved as a repository for future reference. Once the index is generated, it can be stored and utilised for data querying. When a query is made, the system searches for relevant segments within the index. These identified document segments are matched with the user's query and transmitted to the GPT model (GPT-3.5-turbo) through the LangChain framework. This process ensures that the response generated by the model is tailored to the specific context of the query, providing personalised answers. The textual responses generated can then be compared in the subsequent step. In this case study, only five questions and answers are described and compared to illustrate the basic methodology. However, this approach is scalable and can be applied to a larger set of questions and an extensive collection of scientific papers, making it transferable to any LCA context.

3.2. RAG-Based Document Retrieval and Augmentation

To improve the results of LLMs, it is crucial to work qualitatively with input, and prompt engineering has been applied in this paper to achieve that. The significance of prompt engineering lies in its capacity to enhance the adaptability and applicability of LLMs across various sectors [51]. Figure 2 illustrates the components of prompt engineering. Techniques such as zero-shot prompting, where the model makes predictions for unseen tasks using general knowledge, and few-shot prompting, where the model generalises from a minimal number of examples, significantly boost model performance. More advanced methods like CoT prompting, which involves breaking down complex problems into intermediate reasoning steps, enable models to excel in various tasks [52].

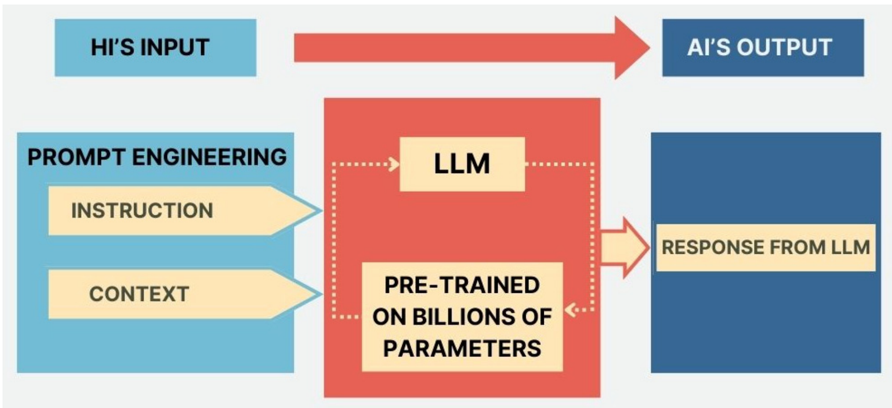

Figure 2. Prompt engineering components adapted from [51].

The CO-STAR framework is a structured approach to goal setting encompassing Context, Outcome, Scale, Time, Actor and Resources, providing clarity and direction in both organisational and personal settings. As per this framework, customised GPT is configured to provide a response based on the following prompt:

> ***(Context)*** *As a research analyst, you are now tasked with answering scientific questions using the literature at your disposal. This requires a deep understanding of the content, the ability to extract relevant information, and the capacity to synthesise this information*

in a manner that directly addresses specific scientific inquiries. ***(Objective)*** *Analyse the scientific papers provided to answer specific scientific questions. Use scientific language and methodologies to ensure your responses are evidence-based and grounded in current research.* ***(Style)*** *Employ a formal scientific writing style characterised by precision, clarity, and thoroughness. Structure your responses with clear argumentation supported by evidence from the literature. Use appropriate scientific terminology and citation practices.* ***(Tone)*** *Maintain a scholarly and objective tone throughout your responses. The tone should reflect the seriousness and rigour typical of scientific discourse, aiming to convey information in a factual and unbiased manner.* ***(Audience)*** *The intended audience for your responses includes scientists, researchers, and academics who are experts in the field. The language and style should cater to an informed audience that expects technical accuracy and depth. Begin each answer by clearly stating the scientific question being addressed.* ***(Response)*** *Review the relevant sections of the provided scientific papers to gather pertinent information and data, synthesise the findings and discuss how they relate to the question at hand, and ensure that all claims are supported by evidence, citing sources in the format: (Author's Name, Year, Article Title), conclude each response by summarising the key points made and their implications for the field of study, recheck the critical studies cited, ensuring that the data reported align with the conclusions drawn and that no crucial information has been misinterpreted or misrepresented in the summary*.

Chain of Verification (CoVe), introduced by Dhuliawala et al. in 2023 [52], aims to mitigate hallucinations in large language models (LLMs) through a systematic four-step process [52]. Initially, the model generates a response, after which it formulates verification questions to assess the accuracy of this response. The model then independently answers these verification questions and revises the initial response based on the verification answers. This process enhances the logical reasoning abilities of the LLM, thereby reducing errors even when faced with contradictory information [52]. This involves generating a baseline response, planning verification questions, answering verification questions independently and producing a revised response incorporating verification. By systematically generating and verifying information through tailored questions, the CoVe method ensures that the output is factual and relevant, significantly reducing the risk of producing hallucinated content. This approach mimics a human-like verification process, enhancing the LLM responses' coherence and reliability.

This method involves using the CO-STAR framework for structured prompt engineering to guide the prompt formulation and leveraging CoVe to enhance response reliability. The goal is to qualitatively assess the performance and answers of these LLMs in generating accurate, relevant and unbiased content for scientific research.

4. Experimental Results and Discussion

In this section, the results of the LLMs are presented, analysed and evaluated. In the first step, Section 4.1 describes the data corpus used for contextual augmentation of the customised ChatGPT in this experiment. Section 4.2 focuses on the questions, where Table 1 presents the responses from different LLMs (customised ChatGPT, ChatGPT-4, Gemini 1.5 and Claude 3.5). Section 4.3 provides an analysis of the responses. Here, the results are interpreted and compared; the comparison of the responses of the different LLMs provides information about the performance of the customised ChatGPT, which were tested by reviewing further questions (Section 4.4). The results from this further investigation, offering a deeper understanding of the customised model, are also presented in Section 4.4.

Table 1. Questions and their responses from LLMs. The table displays questions and corresponding answers from three LLMs compared with optimised GPT. Some of the answers in the table are represented by abbreviations of methods, with their full names listed in the last row of the table.

Question 1	What Machine Learning (ML) Approaches are Suitable for Collecting Life Cycle Inventory (LCI) Data for a 5 MW Inverter Used in Proton Exchange Membrane Water Electrolysis (PEMWE) When Existing Databases Lack This Information?	
Customised Chat GPT	Answer	ANNs can model complex relationships and predict missing data by learning from available related datasets. In the context of PEMWE Life Cycle Assessment (LCA), where detailed and accurate LCI data are crucial, ANNs can fill gaps in the inventory, ensuring a more comprehensive and reliable environmental assessment of the PEMWE system.
	References	Khoshnevisan, B., Rafiee, S., Omid, M., Mousazadeh, H. and Sefeedpari, P. Prognostication of environmental indices in potato production using artificial neural networks. 2013 [53]
Chat GPT-4o	Answer	Data Augmentation: Regression analysis, support vector machines, or ANN with synthetic data generation or transfer learning. Clustering: K-means or hierarchical clustering. Hybrid approaches: support vector machines or generative models.
Gemini 1.5	Answer	Regression or random forest
Claude 3.5	Answer	Predictive modelling, transfer learning, generative adversarial networks, variational autoencoder and natural language processing.
Question 2	What machine learning methods can be applied to rectify overestimated environmental impact data of copper in LCI databases?	
Customised Chat GPT	Answer	Support vector machines or random forest. Machine learning methods such as support vector machines (SVM) or random forests can be applied to rectify overestimated copper environmental impact data in Life Cycle Inventory (LCI) databases. These techniques effectively identify and correct anomalies by learning from patterns within the data, leading to more accurate environmental assessments.
	References	Omidkar, A., Alagumalai, A., Li, Z. and Song, H. Machine learning assisted techno-economic and life cycle assessment of organic solid waste upgrading under natural gas. 2024 [54]
Chat GPT-4o	Answer	Data imputation: Linear regression, ridge regression or gradient boosting machines. Anomaly detection: Isolation Forest, variational autoencoder or principal component analysis. Ensemble learning: an ensemble of regression and anomaly detection models.
Gemini 1.5	Answer	Regression model
Claude 3.5	Answer	Isolation forest, support vector machines, random forest with gradient boosting machines, gaussian process regression, multi-task learning, Bayesian ML models with data or expert opinions.
Question 3:	Which Life Cycle Impact Assessment (LCIA) methods are recommended for conducting a Life Cycle Assessment (LCA) of Proton Exchange Membrane Water Electrolysis (PEMWE) systems, and why?	

Table 1. *Cont.*

Question 1	What Machine Learning (ML) Approaches are Suitable for Collecting Life Cycle Inventory (LCI) Data for a 5 MW Inverter Used in Proton Exchange Membrane Water Electrolysis (PEMWE) When Existing Databases Lack This Information?	
Customised Chat GPT	Answer	CML 2001 provides a well-established framework for midpoint impact categories, allowing for detailed environmental impact analysis, especially in areas like resource depletion and global warming. ReCiPe offers both midpoint and endpoint impact assessment, making it versatile for capturing various environmental impacts, including human health and ecosystem quality. TRACI is particularly relevant for assessments within the United States. It focuses on region-specific impact categories, such as smog formation and acidification, which are important for evaluating PEMWE systems in that context.
	References	Algren, M., Fisher, W. and Landis, A. E. Machine learning in life cycle assessment. 2021 [55]
Chat GPT-4o	Answer	ReCiPe, ILCD and TRACI
Gemini 1.5	Answer	CML, TRACI, ReCiPe and IMPACT 2002+
Claude 3.5	Answer	ReCiPe, CML, ILCD, USEtox, IPCC GWP
Question 4:	How can machine learning be utilised to conduct a sensitivity analysis on the LCIA results of a PEMWE system?	
Customised Chat GPT	Answer	Random Forest: • Efficiently handles complex and non-linear relationships in LCIA data. • Identifies and ranks the most influential factors affecting the environmental impact of PEMWE systems. Gradient Boosting Machines: • Provides precise sensitivity analysis by incrementally improving predictions on LCIA outcomes. • Highlights key parameters that significantly influence the overall environmental performance of PEMWE systems, allowing for targeted optimisations.
	References	Omidkar, A., Alagumalai, A., Li, Z. and Song, H. Machine learning assisted techno-economic and life cycle assessment of organic solid waste upgrading under natural gas. 2024 [54] Zheng, L., Mueller, M., Luo, C. and Yan, X. Predicting whole-life carbon emissions for buildings using different machine learning algorithms: A case study on typical residential properties in Cornwall. 2024 [56]
Chat GPT-4o	Answer	ANN trained on monte-carlo simulation. Random Forest or gradient boosting machines.
Gemini 1.5	Answer	Gaussian process regression and ANN
Claude 3.5	Answer	Random forest or gradient boosting machines, Sobol in-dices, variational autoencoders, optimise neural networks or Gaussian process, t-SNE (t-distributed Stochastic Neighbour Embedding) and UMAP (Uniform Manifold Approximation and Projection), polynomial chaos expansion or kriging.
Question 5:	How can machine learning assist in generating optimised recommendations based on LCIA results for Proton Exchange Membrane Water Electrolysis (PEMWE) systems?	

Table 1. *Cont.*

Question 1	What Machine Learning (ML) Approaches are Suitable for Collecting Life Cycle Inventory (LCI) Data for a 5 MW Inverter Used in Proton Exchange Membrane Water Electrolysis (PEMWE) When Existing Databases Lack This Information?	
Customised Chat GPT	Answer	Artificial Neural Networks (ANNs): Learn complex patterns in PEMWE performance and environmental impact data, enabling accurate predictions and optimisations. Genetic Algorithms: Optimise the structure and parameters of ANNs, enhancing their ability to find the best PEMWE configurations for minimal environmental impact. Bayesian Optimisation: Efficiently tunes ANN parameters by focusing on the most promising areas, improving PEMWE performance and reducing environmental impacts in line with LCIA findings.
	References	Omidkar, A., Alagumalai, A., Li, Z., and Song, H. Machine learning assisted techno-economic and life cycle assessment of organic solid waste upgrading under natural gas. 2024 [54] Kaab, A., Sharifi, M., Mobli, H., Nabavi-Pelesaraei, A., and Chau, K. W. Combined life cycle assessment and artificial intelligence for prediction of output energy and environmental impacts of sugarcane production. 2019 [57]
Chat GPT-4o	Answer	Genetic algorithms, Particle swarm optimisation and simulated annealing. Multi-objective evolutionary algorithms. Predictive modelling with decision support systems.
Gemini 1.5	Answer	Gaussian process regression and ANN
Claude 3.5	Answer	Non-dominated sorting genetic algorithm II or multi-objective evolutionary algorithm based on decomposition. Deep Q-networks; K-means or hierarchical clustering with support vector machines and random forest. Gaussian process Bayesian optimisation, collaborative filtering, casual forest, Shapley additive explanations or local interpretable model-agnostic explanations.

ILCD: The International Reference Life Cycle Data System, TRACI: Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts, USEtox: The Toxicity Model from the Society of Environmental Toxicology and Chemistry of Environment Programme of United Nations.

4.1. Description of the Data Corpus for Augmentation

In this paper, the custom GPT model was tested against the responses from three other large language models: OpenAI's ChatGPT-4o, Gemini 1.5 and Claude 3.5 because they have demonstrated significant potential in scientific research. One of the unique features of OpenAI is the ability to create a customised GPT, which in turn provides the ability to apply a specific library of scientific literature to teach an LLM for a particular use case.

In this research, a customised ChatGPT model was developed to provide expert insights at the intersection of ML, LCA and hydrogen technologies. To train this model, a focused literature review was conducted using the Scholar database. The search targeted key areas using keywords such as "PEMWE", "Environmental impact" and "Machine learning in LCA". The final data corpus included 39 research papers, carefully selected for their relevance. This selection comprised 10 papers on LCA methodologies, 3 systematic reviews and 26 papers focused on the application of ML in LCA. The systematic reviews were particularly important, covering challenges and future needs in PEMWE technology, advancements in applying ML to LCA and the life-cycle assessment of hydrogen technologies. The information for these papers can be found in the Supplementary Materials.

The three selected review papers focus on key areas relevant to the intersection of machine learning, life cycle assessment and hydrogen technologies. The first paper discusses the challenges and future needs of PEMWEs, which are crucial for hydrogen production.

The second paper reviews the advancements in ML to LCA, highlighting current trends and challenges in this field. The third paper examines the LCA of hydrogen technologies, with an emphasis on critical raw materials and sustainability, particularly in the context of end-of-life strategies. The 26 papers focused on the application of ML in LCA were selected by using the keywords 'Machine Learning' AND 'Life cycle assessment', 'hydrogen production', 'PEMWE', 'Artificial Intelligence'. The 10 papers on LCA methods were selected by using the keywords 'LCA' AND 'PEMWE', 'LCA' AND 'hydrogen production'.

Gemini and Claude are not able to analyse many papers because they have limitations on the number of tokens. The customised LLM comprehends instructions by extracting relevant techniques, algorithms and methodologies from the provided literature. It then synthesises this information to provide practical recommendations for optimising LCA with ML algorithms, ensuring accuracy and efficiency improvements. This distinguishes it from other models and, therefore, requires separate consideration.

4.2. Formulation of Queries

One of the main objectives of this paper is to analyse the extent to which LLM can help solve complex challenges at the interface of ML, LCA and of ML, LCA and PEMWE. For this reason, the various questions asked to the LLMs arise from the challenges described in Sections 2.2 and 2.3. To enable a comparison of the answers, the four LLMs were asked the same questions. The questions were prompted into the pipeline and then evaluated, taking the reference answers into account. The list of questions is as follows:

1. What machine learning (ML) approaches are suitable for collecting Life Cycle Inventory (LCI) data for a 5 MW inverter used in Proton Exchange Membrane Water Electrolysis (PEMWE) when existing databases lack this information?
2. What machine learning methods can be applied to rectify overestimated environmental impact data of copper in LCI databases?
3. Which Life Cycle Impact Assessment (LCIA) methods are recommended for conducting a Life Cycle Assessment (LCA) of Proton Exchange Membrane Water Electrolysis (PEMWE) systems, and why?
4. How can machine learning be utilised to conduct a sensitivity analysis on the LCIA results of a PEMWE system?
5. How can machine learning assist in generating optimised recommendations based on LCIA results for Proton Exchange Membrane Water Electrolysis (PEMWE) systems?

The first question focuses on challenges that have already arisen in conducting an LCA for PEMWE in Section 2.3 and aims to explore which ML techniques can be provided by trained LLMs to address these challenges. The second question relates to the general challenges of data gaps, as described in Section 2.2. Questions three to five aim to check how LLMs can respond to and assist with general LCA problems when they occur in the context of PEMWE. For reasons of clarity, the five questions were formulated so that a comparison of the 20 answers from the different LLMs can be presented in a table. The answers of the different LLMs are shown in Table 1.

4.3. Analysis of the Responses

In this section, the analysis of the responses is conducted by interpreting and comparing the variations among the different answers.

In response to Q1, the customised GPT concludes that employing ANNs is a rational approach for estimating missing data in the LCI of PEMWE. Although the response initially draws from an agricultural example, the model adapts this knowledge to the context of PEMWE. This demonstrates the model's capability to synthesise insights across the three intersecting fields of ML, LCA and PEMWE. Upon manual fact-checking, the conclusion can be validated as accurate, since the application of ANNs in PEMWE is well-supported in the scientific literature [58]. In response to Q2, the customised GPT suggests using SVM or RF to rectify overestimated data. After manual verification, this suggestion is found to be valid, as it aligns with conclusions from relevant scientific articles in this domain [59,60]. For Q3, the model recommends three methods for assessing environmental impact: CML, ReCiPe and TRACI. However, it overlooks that the CML database has not been updated since 2017 [61] and TRACI has geographical limitations [62]. Furthermore, the model does not clearly define the boundaries between these methods, relying instead on listing them in succession from the cited article. While the recommendation is not entirely accurate, it still provides a useful starting point, as these are commonly applied methods. The answer to Q4 can be deemed correct, as it is consistent with current theories in the field, as noted previously. However, evaluating the correctness of the response to Q5 is more challenging, as it is primarily designed to offer recommendations. In this case, GPT synthesises information from both the uploaded data and its own internal databases, tailoring the output to the PEMWE context specified in the prompt. Overall, the customised GPT demonstrates the ability to generate answers by synthesising data from various sources, but the accuracy of its responses is dependent on the quantity of input data and the clarity of the questions posed. This underscores the importance of well-structured queries and sufficient data to guide the GPT in generating reliable and context-specific answers.

Notably, manual fact-checking is essential to verify the accuracy of LLM-generated responses, ensuring that the synthesis of information from heterogeneous sources—such as ML, LCA and PEMWE—corresponds to established facts. In this context, it is important to differentiate between two types of LLM responses: synthesised and generative. Synthesised responses strictly contain information extracted from the training data without modification, accurately reflecting the provided references. On the other hand, generative responses are derived from the given data, but GPT introduces additional connections or insights that extend beyond the explicit content of the training data, creating links between the provided information and the specific context of the task. These generative responses, while potentially insightful, require closer scrutiny, as they are not always directly grounded in the literature. Based on the above distinctions, the responses to question 1, 2 and 4 in Table 1 are generative, while the responses to question 3 and 5 are synthesised. As the results of comparing different types of responses show, purely synthesised responses are reliably answered through information extraction. However, for generative responses, the processing of information and the generation of links must be further tested to ensure the proposed answers.

The differences in the responses of LLMs can be attributed to their distinct training databases, fine-tuning techniques and intended application contexts. These variations impact their ability to provide practical details, categorise methods and cite literature. The customised ChatGPT provided specific examples of machine learning methods, emphasising their practical applications and summarising their documented uses in the literature. For example, random forests were suggested for correcting overestimated copper environmental impact data in LCI databases, and ANNs were recommended for estimating missing technical data in PEMWE systems. This customised ChatGPT is tailored to deliver example-driven explanations, indicating an optimisation for scenarios that require clear, direct demonstrations of ML methods. However, ChatGPT-4o categorised several machine learning methods, provided reasons for their selection, and illustrated one solution in an application context, but it lacked practical details and literature citations. For instance, it mentioned regression and random forest as methods for predicting missing technical data in PEMWE, but did not delve into the reasoning or processes behind these methods, as shown in Table 1. This approach is beneficial for users looking to understand the broader landscape of ML methods applied to the LCA of PEMWE, rather than for those seeking detailed application guidance. The absence of practical details and citations could reflect a focus on conceptual clarity and method variety over depth, or it might indicate a trade-off made to prioritise breadth over detailed practical guidance. Unlike customised GPT, other GPTs are trained on massive internet data, open sources such as Wikipedia articles and articles on various websites [63]. Gemini 1.5 referenced machine learning methods with citations but lacked practical explanations, suggesting its design prioritises providing quick references and illustrating applications through the literature. This version seems suited for users who need to rapidly locate relevant studies without requiring detailed explanations or step-by-step guidance. In contrast, Claude 3.5 categorised and explained various ML methods to address specific questions, especially emphasising practical approaches for questions 4 and 5. However, it did not include literature citations, indicating a focus on delivering immediate, actionable insights rather than academic references. This suggests Claude 3.5 is optimised for context-driven queries that prioritise practical solutions.

The customised ChatGPT is a RAG-LLM model, whose strength lies significantly in the quality of the curated documents used as the foundation for generating the responses. The customised GPT model provides answers by integrating various perspectives, methodologies and findings by synthesising across multiple documents. The curation process ensures that the LLM is equipped with highly relevant and domain-specific information, which inevitably contributes to its improved performance over off-the-shelf LLMs.

The customisation of LLMs described here is primarily user-centric, tailored to address specific problems and application needs rather than providing a broad academic overview. This customisation process involves trade-offs that are aligned with the user's particular requirements and the context of the application. The focus can vary, placing emphasis on practical details, the categorisation of methods or the citation of relevant literature, depending on the intended use case and user priorities. Understanding these focus areas is crucial for selecting the most appropriate LLM version for specific research and practical applications. It ensures that the model achieves an optimal balance between theoretical insight, practical utility, and academic rigour, thereby effectively meeting the needs of its intended users.

At this point, it should be noted that there are a variety of ways to ask questions about the challenges and that this can have an impact on the answers. However, as the focus is initially on comparing the different LLMs and the questions asked of the different LLMs remain the same, the specific nature of the question is less scrutinised in the responses to Table 1. Nevertheless, it must be recognised that this could present a limitation that must be considered. Given the assumptions that (1) a synthesised response will be generated based on the information in the training data, and (2) if the information is included in the training data, the customised GPT should be able to locate it and provide the corresponding source, the assumptions drawn from the answers to the five questions in Table 1 should be tested again in the next section with the help of additional questions.

4.4. Further Investigation LLM Responses

In this section, the assumptions drawn from Section 4.3 are tested. The customised ChatGPT was trained on the same 39 research papers mentioned in Section 4.1. This time, however, five papers were randomly selected from this pool. After thoroughly reading these articles, the following five questions were formulated based on their content. The purpose of this approach was to ensure that the questions were designed such that the answers could be found within the articles. The questions posed were as follows:

1. What are the main differences between supervised and unsupervised machine learning, and how can each be applied to different stages of a Life Cycle Assessment (LCA)? Source [64]
2. How do machine learning models, such as Artificial Neural Networks (ANNs) handle non-linear relationships in environmental impact predictions, and what are their advantages over traditional regression models? Source [65]
3. In multi-objective optimisation using LCA, how does the Pareto-optimal solution help in balancing trade-offs between competing environmental and economic goals? Source [66]
4. What are the main limitations of using traditional LCA methods without the incorporation of machine learning, and how do ML approaches address these limitations? Source [64]

5. How does the use of ML algorithms, such as decision trees and deep learning, improve the characterisation factor (CF) estimations in LCAs involving complex and dynamic systems? Source [67]

The responses to these questions are presented in Table 2.

Table 2. The table shows the results of responses of the customised GPT to questions expecting a synthesised response from the training literature.

Question 1S	What are the Main Differences Between Supervised and Unsupervised Machine Learning, and How Can Each be Applied to Different Stages of a Life Cycle Assessment (LCA)?	
Customised Chat GPT	Answer	Supervised learning uses labelled data to train models, making it ideal for predicting specific environmental impacts in LCA by associating inputs (e.g., material usage) with outputs (e.g., emissions). In contrast, unsupervised learning is applied to discover patterns or groupings in datasets without predefined labels, such as clustering similar products based on their environmental impact profiles. Both methods can be employed to improve data accuracy and interpret LCA results [64,68].
Question 2S	How do machine learning models, such as Artificial Neural Networks (ANNs) handle non-linear relationships in environmental impact predictions, and what are their advantages over traditional regression models?	
Customised Chat GPT	Answer	Artificial Neural Networks (ANNs) excel at modelling complex, non-linear relationships between inputs and outputs in LCA due to their capacity to learn from large datasets and capture hidden dependencies. Traditional regression models, while useful for linear relationships, often fail to accurately predict environmental impacts when non-linearities are involved. ANNs and RF models are more flexible and can achieve higher prediction accuracy in such cases [65].
Question 3S	In multi-objective optimisation using LCA, how does the Pareto-optimal solution help in balancing trade-offs between competing environmental and economic goals?	
Customised Chat GPT	Answer	The Pareto-optimal solution in multi-objective optimisation helps balance trade-offs by identifying a set of non-dominated solutions, where improving one objective (e.g., reducing environmental impact) cannot be achieved without worsening another (e.g., increasing costs). In LCA, Pareto-optimal solutions allow decision-makers to evaluate the trade-offs between environmental and economic goals and select the most balanced option [66,69].
Question 4S	What are the main limitations of using traditional LCA methods without the incorporation of machine learning, and how do ML approaches address these limitations?	
Customised Chat GPT	Answer	Traditional LCA methods rely heavily on manual data processing and can struggle with incomplete datasets or complex systems with non-linear dependencies. ML approaches overcome these limitations by automating data processing, filling gaps in life cycle inventories and improving prediction accuracy for complex, non-linear systems. ML also allows faster processing of large datasets, which significantly reduces the time required for LCA computations [64,68].
Question 5S	How does the use of ML algorithms, such as decision trees and deep learning, improve the characterisation factor (CF) estimations in LCAs involving complex and dynamic systems?	
Customised Chat GPT	Answer	ML algorithms like decision trees and deep learning improve CF estimations in LCAs by accurately modelling the relationships between various environmental factors, such as material usage, energy consumption and emissions. These algorithms can process large amounts of data and account for the dynamic interactions between different life cycle stages, leading to more precise CF estimations. They are especially useful in scenarios where traditional methods might oversimplify or miss key dependencies [67].

S—Synthesised Response.

The answers provided by the customised GPT demonstrate that it identified and located relevant sources for the previously asked questions. For example, in question 2S, the exact source [65], was correctly identified and cited in response to the question, confirming that the source being searched for was found. For question 5S, source [67] provided a detailed explanation of using decision trees and other methods to build ML models for estimating hazardous concentrations and determining ecotoxicity characterisation factors, which directly addressed the question. This structured approach shows how the customised GPT handled the questions and identified the relevant sources for most answers, while also highlighting areas where multiple sources were likely used to enhance the accuracy of the response. However, there were some anomalies in questions 1S, 3S and 4S. Initially, the answers did not directly reference a specific source. In the case of question 1S, source [64] was referenced, which primarily focuses on machine learning (ML) with only a minor section on life cycle assessment (LCA). It seems that source [68] was likely used to verify the LCA components of the response, ensuring the relevant aspects of the question were covered. In question 3, the response mentioned "improving one objective cannot be achieved without worsening another", which was directly linked to source [66]. Additionally, source [70] was cited for discussing the use of the Pareto front to visualise LCA. However, while source [70] mentions the Pareto front, its relevance to the question is much less significant compared to the insights from source [66]. Overall, the assumptions that were already made in Table 1 can be regarded as confirmed. The findings in Tables 1 and 2 indicate that LLMs have already contributed, to some extent, to assisting LCA professionals in using ML to provide new impulses to address potential challenges in LCA.

5. Conclusions

This study investigates using artificial intelligence as a customised, large-scale language model to improve LCA. The aim is to improve the challenges of environmental impact assessment, such as data gaps, as described in the use case of green hydrogen by PEMWE. By integrating advanced LLM capabilities, the method proposed in the study provides a robust tool for resolving specific and general issues within LCA practice. The applicability of this approach improves the reliability of LCA results and optimises the research process by reducing the time and resources required for data analysis. Additionally, the customised LLMs can offer problem-solving guidance through further queries and relevant citations, providing assistance to LCA researchers without a background in ML.

The findings of this paper indicate that customised LLMs can analyse and synthesise information from a diverse set of sources, significantly aiding researchers in navigating the complexities of LCA by providing qualitative insights and identifying suitable ML solutions. As demonstrated by the results, customised LLMs can offer advice on selecting LCIA methods, suggest ML techniques for sensitivity analysis and recommend environmental optimisation strategies for PEMWE. These contributions, using PEMWE as an example, demonstrate how LLMs can help to address the general challenges faced in LCA, as discussed in the paper, by providing clear, actionable insights and facilitating easy interaction with the LLM will enhance its utility for practitioners with varying levels of expertise.

This research also shows the importance of prompt engineering in optimising LLM performance. By tailoring the prompts for comparative analysis, it was ensured that the LLM-generated responses were precise, clear and grounded in current research, effectively catering to an informed audience of scientists and researchers. The questions in Section 4 were designed to directly address the challenges inherent in LCA, as well as those specific to PEMWE. Recognising that the formulation of prompts significantly influences responses, open-ended questions were deliberately chosen. This approach allows for a wide range of potential answers, providing a broad spectrum of insights. However, the trade-off is a reduced likelihood of receiving highly specific responses.

The results of the LLM customised with scientific articles were validated and verified against scientific research data in the specific field of PEMWE even though the original literature base did not include articles containing the inferences drawn. In contrast to customised models, non-customised models are not as reliable due to their underlying database, which often contains irrelevant data due to its shallow depth. Moreover, it is worth noting that, the customised LLM generates two types of responses in this study: synthesised responses and generative responses. Synthesised responses adhere to the information provided in the training data, making this type of response trustworthy. In contrast, generative responses are based on the training data but involve a certain level of inference by the LLM, indicating that these responses need to be re-evaluated by manually checking.

Future work can focus on refining the training of LLMs with more specific and up-to-date datasets related to PEMWE and other green hydrogen technologies, as well as fundamental LCA-related literature, such as the ILCD handbooks, the textbook from Hauschild et al. [71] etc. Also, future studies should consider training GPT on data from practical applications of machine learning in LCA to explore LLM as a tool to provide not only theoretical information but also practical guidance. Although RAG enhances the retrieval of the most pertinent sections from the curated corpus, future improvement might involve automating parts of the document selection process. This could lessen the dependence on manual curation, making the system more scalable and potentially reducing the need for highly selective document retrieval. To enhance the precision and relevance of the answers, future work should also focus on refining prompts through advanced prompt engineering techniques. For instance, tailoring questions to target specific LCA challenges with greater granularity can increase the likelihood of eliciting more focused and actionable responses from the LLM. Additionally, incorporating strategies such as Tree-of-Thought or Chain-of-Thought reasoning could further improve the depth and coherence of the model's responses, enabling it to address complex questions more effectively. Additionally, ongoing collaboration between AI and domain experts is essential to continuously validate and enhance the outputs generated by LLMs. By addressing the ethical considerations and biases inherent in AI models, the responsible and effective use of LLMs in scientific research can be further ensured.

In conclusion, integrating LLMs into the LCA process marks a significant step towards creating a solution for using ML in LCA and improving it. This approach demonstrates that AI can provide powerful tools for advancing research in renewable energy and sustainability.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/make6040122/s1. References [7,16,17,23,24,28,29,35,53–57,68,70,72–95] are cited in the supplementary materials.

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