
Developing a curated chatbot as an exploratory communication tool for chemistry learning

Annabelle T. Lolinco, Thomas A. Holme*

Department of Chemistry, Iowa State University, Ames, IA 50011

ABSTRACT

In a technology-centric world, leveraging digital tools such as chatbots allows educators to engage students in ways that may be more accessible for both parties, particularly in large lecture classrooms. This report details the development of an interactive web-based chatbot to curate content for writing about chemistry in context. Students were assigned a 500-word paper where they discuss general chemistry concepts through the lens of a timely, sustainability-related topic, i.e., water footprint, carbon footprint, or embodied carbon. Using machine learning, the chatbot underwent training through the phrases inputted by the developer and its users to create stronger connections to different options for users to switch to at will. Discussed herein are the development of the decision tree, the chatbot's components, and results from the initial implementation in a large lecture general chemistry classroom. Over 78% of the 347 enrolled students (271) used the chatbot over 350 times in the three weeks leading up to the assigned due date of the paper. 83% of the interactions were captured for further analysis, which showed that 22% of students used the chatbot more than once. 46% of recorded interactions were used to aid students in developing or refining their idea for the assignment. The curated chatbot technology reported here for writing assignments in chemistry can be readily adapted to other aspects of coursework in chemistry.

GRAPHICAL ABSTRACT



25 **KEYWORDS**
 Digital Assistant, Student Writing, Rich Context, Interdisciplinary, Applications of Chemistry, First-Year

30 **INTRODUCTION**

Digital conversations are not just between humans these days. In fact, programmed virtual assistants can take on the conversational burden of answering routine queries such as finding the status of a package. Chatbots are one specific branch of virtual assistants that only require natural language processing and interpretation as opposed to the more integrated, voice-activated, and processed smart assistants such as Apple's Siri or Amazon's Alexa. Chatbots have been used for queries since the 1960s, with the world's first chatbot being ELIZA¹. Modern chatbots leverage the advances of machine learning and the natural language processing training to recognize key phrases to activate modules that are responsive to user inputs. Over the years, research on chatbots and its capability in sectors such as commerce²⁻⁷, health^{8,9}, and education¹⁰⁻¹⁷ captured use cases and how to

40 leverage them. However, there is still more to explore within the context of science learning and the support of students' more personalized engagement with digitized tools.

The utility of chatbots in education and education research has manifested through studies on critical thinking of knowledge acquired and learner engagement. For the former, assessments can be readily measured for topics such as learning a language^{13,17-20} and other technical and practical
45 skills^{14,16,21}. Within chemistry, chatbots have been implemented to prepare students for formal assessments as detailed by Korsakova et. al.²² While comparative studies show mixed results of students learning more with chatbots, research has shown that chatbots keep students engaged^{11,23,24}. When online distance learning significantly increased due to the onset of the COVID-19 pandemic, the use of digital tools, including chatbots, also increased. In fact, with the emergence of generative
50 artificial intelligence informing chatbots such as ChatGPT, studies on the impact and extent of digital assistance in education have become a central topic.²⁵⁻³¹ Other efforts in the science education community have used machine learning and software tools to provide feedback or assessment for writing experiences.³²⁻³⁵ However, the instructor curated content for chatbots described in this paper expands on the understanding of how students use this tool to explore course content.

55 The impetus of building a chatbot for the chemistry classroom began with the aim to provide an automated and responsive tool that could reach many more students in a large lecture course than is feasible for the numerically small instructional staff. The writing piece assigned is a 500-word essay that connects the general chemistry content explored in the course to a broad sustainable-related context that is timely and could suit students' varied interests (see Supporting Information – Item 1).
60 The implementation of the chatbot was deployed in a first-semester general chemistry course at a large U.S. research university, where enrollment was 347 students from the life and physical sciences. Additionally, a curated chatbot can be a tool to narrow the vast amount of information at students' disposal by prioritizing the discovery by students of vetted and valuable information. From an instructional research perspective, the chatbot's logs allow an instructor to gain insight into the
65 choices students make in generating a formal piece of writing. This paper details the development and

initial uses of a chatbot providing information to connect topical sustainability and chemical information for a written paper assigned to students taking General Chemistry.

DEVELOPMENT PROCESS

70 The development of curated chatbots used in the large lecture-style classroom stemmed from initial research in student engagement with contextualizing chemistry through writing. An initial intervention where students voluntarily met with an expert facilitator in a one-on-one session, a soundboard, was an opportunity to talk and map out students' approach to the writing assignment, 75 based on results from studies on generative learning^{36,37} and writing-to-learn practices^{38–42}. Artifacts from the students' experiences in the soundboard sessions led to discoveries of common concerns which informed efforts to automate experiences via the programming of virtual assistants or chatbots. Thus, chatbot outputs were patterned on information derived by in-person writing assistance efforts and informed a curation process that emphasized solutions to common student challenges.

80 Given the advances in technology, a chatbot does not need to be written from the ground up. Tools such as Microsoft Virtual Power Agents⁴³ and IBM Cloud's Watson Assistant⁴⁴ are viable ways to adapt chatbots. The chatbot described herein was developed natively in IBM Cloud's Watson Assistant tool; the user interface was designed so that no coding was necessary to leverage the tool's machine learning capabilities. Those familiar with programming can go further and work with Java in the 85 platform's coding interface. What is necessary to develop a curated chatbot is the decision tree and its branches of choices a user may utilize.⁴⁵

Patterns of student interests and challenges found through the soundboard sessions were used to identify typical questions students have when asked to write about chemistry within the rich context of sustainability. Those patterns provided data upon which an initial decision tree could be postulated. 90 A truncated example of such patterns is provided in the form of a partial decision tree in Figure 1.

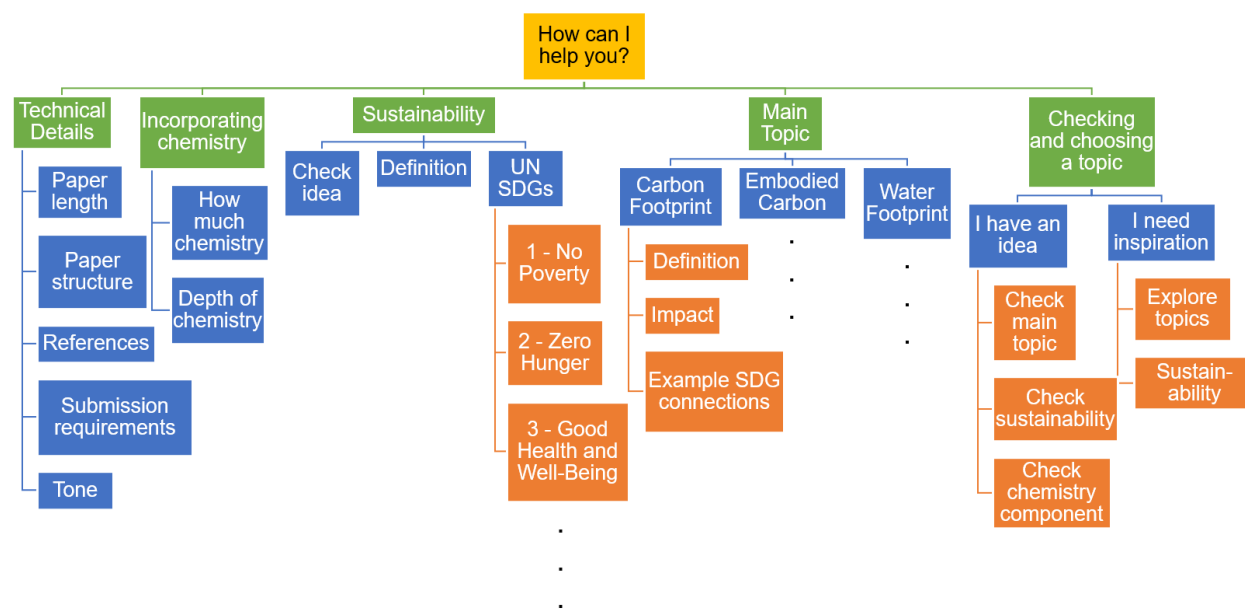


Figure 1: Truncated decision tree for a chatbot related to student writing about chemistry and sustainability.

This decision tree representation was designed to highlight key factors that provide specific values to students. For example, some number of students required practical information such as assignment parameters like format, word limits, etc. Such utilitarian queries arose from students' need to confirm the technical details of how to complete the assignment to the specifications given by the instructor (far left). Other aspects of the writing assignment emphasized more exploratory activities, such as how to start picking a paper topic (2nd from right – main topic). Some students accessed the chatbot with very nebulous ideas for how to approach the assignment. Thus, the decision tree included a bounded exploration for students to use in identifying their writing questions (far right). In the Fall 2021 semester, students had the option to write about chemistry in the context of water footprint, carbon footprint, or embodied carbon. Therefore, the decision tree included modules providing the definitions, a broad range of impacts, and connections to sustainability issues regarding those three areas. This structure guided students into assigned areas of context and gave them the ability to pick where they wanted to go. Given the machine learning capabilities embedded in the chatbot systems, training phrases aided the chatbot's recognition of student-typed responses to the correct topic of interest.

Thus, users could explore regardless of whether it was chatbot-guided or self-driven. A detailed navigation document for the chatbot can be found in Supporting Information (Item 2).

110 In addition to the practical benefit of helping students complete a writing assignment, the students' interactions with a chatbot can be logged, and served as a formative assessment for the instructor. There are two items available in the user logs: an *action* and a *step*. *Actions* describe the user actions related to a specific content area. A helpful synonym for an action could be "module". *Steps* are a count of how many separate text inputs, or user actions, take place within one *action*.

115 Consider the "carbon footprint" action in Figure 1. Within that action, students have several choices that include learning more about the definition, impact or ways carbon footprint can connect to sustainability. Any given user of the chatbot may take one, or many, actions and each would be identified as a step within the carbon footprint action. The machine learning aspect for this type of curated chatbot represents a key mechanism by which users transition between actions. This style of
120 interaction depends on the exploratory nature of the chatbot. At any point, a user may type in a phrase. When this new phrase or query, known as a trigger phrase, can be matched to a phrase that the chatbot recognizes through its machine learning capacity and transition to a new portion of the decision tree. While a chatbot can be expansive, the goal of using this tool is not to provide direct solutions for the student user. Rather, the chatbot gave the student opportunities to explore curated
125 information which they knew is related to what they are learning.

To elaborate further on the nature of steps and actions, Figure 2 presents a portion of a hierarchical structure, showing at least two different types of actions. Looking at sustainability, a student who clicks on the option to see the definition has entered that action. There are no substructures there, so a typical action with the definition will likely have only one step. If, however,
130 the student was interested in learning more about UN Sustainable Development Goals (UNSDGs), particularly Goal 3, there are multiple steps within that single UNSDG. Each step may provide details about the topic and then spawn a query for the user. For the sake of clarity, users see the individual steps altogether until a prompt. In this case, after a user explores the UNSDG3 as thoroughly as desired, the chatbot asks if they wish to explore other UNSDGs.

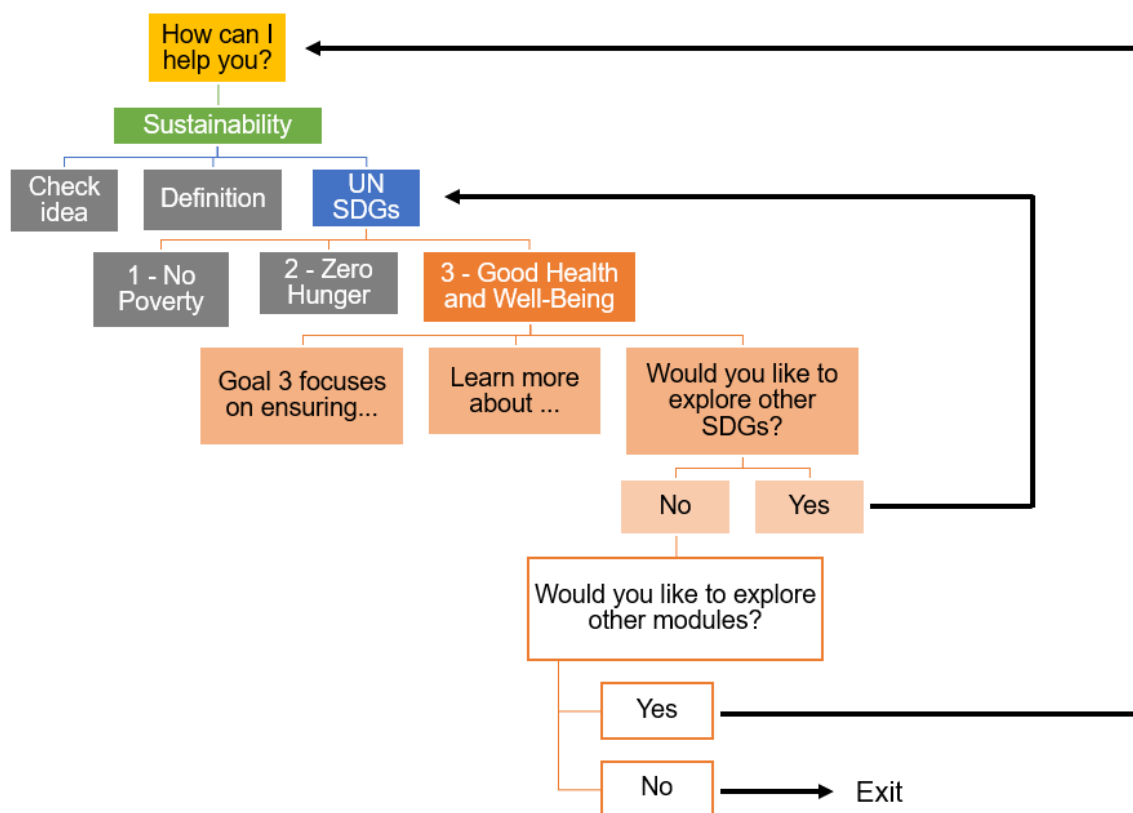


Figure 2: Illustration of the development of inquiry granularity for a portion of the chatbot covering the United Nations Sustainable Development Goals. Exploration within the UNSDGs action is more extensive than what is possible within the Sustainability's Definition action, which has a singular step in comparison.

An analysis of the logbook of users' interactions revealed the steps participants used in the chatbot and actions enacted in the chatbot. Additionally, logistical information, such as time spent with chatbot before disconnecting, date and time used were captured and used for subsequent analysis. A brief participant interaction constructed from log files is provided in Box 1. In this example, the student asked about a technical requirement for the paper which was quickly answered. Given the chatbot-initiated query to explore further, the student agreed and their second action, to check their ideas for the paper content, explored several capabilities of the chatbot about the content and context of the assignment.

Box 1: Detailed mock-up of the log of a student – chatbot interaction where the student interactions are highlighted to differentiate from the text the chatbot provides (based on actual participant interactions, but not from a specific participant).

Chatbot Log Example

Participant 035

Interaction 001

10/13/2022

0120 – 0125

Would you like to see the ways I can help? → Yes

-Top help → Technical requirements

-Technical requirements → Paper length

-Would you like to explore more technical requirements? → No, I don't want to see technical requirements

-Would you like to explore other topics? → Yes, I would like to see the ways you can help

- Top help → Checking and choosing a topic

- Do you have an idea or need some inspiration? → I have an idea

- Does your idea cover one of the main topic ideas? (Water footprint, carbon footprint, or embodied carbon → Yes

-Does your idea also incorporate some element of sustainability? → No

-Finally, did you include some tie to chemistry? → Yes

Looks like you're missing a component or two. What area would you like to get more information about? → Sustainability

- Sounds like you need help with sustainability. Do you want to review the definition of sustainability, explore the United Nations' Sustainability Development Goals, or check your idea of sustainability for your paper? → UN SDGs

- There are 17 different UN sustainable development goals (SDGs). You can incorporate one, or more, in your paper. Which one would you like to explore? → SDG 6 – Clean Water and Sanitation

Would you like to explore the other SDGs? → Yes, other SDGs

-Which one would you like to explore? → SDG 12 – Responsible Consumption and Production

What would you like to explore next? → I'm done

End

IMPLEMENTATION

A curated chatbot²⁸ was developed and used in a large lecture general chemistry course at an R1 university to aid in a writing assignment. The prompt was to connect chemistry and sustainability under a specific topic, in this case, either water footprint, embodied carbon, or carbon footprint, within 500 words. Students were given free rein and access to the chatbot as a tool approximately three weeks prior to a written assignment's deadline and could use this tool as needed. The chatbot was presented as a curated tool that had information to help one start to think about the assignment as well as provide some avenues to explore and checkpoints to aid in the writing process. In the pilot implementation, 271 unique students, in a class size of 347 (78%) used the chatbot 352 times over the 21 recorded days. The additional analysis provided here is for students' usage patterns.

Observations of student interactions with the Chatbot

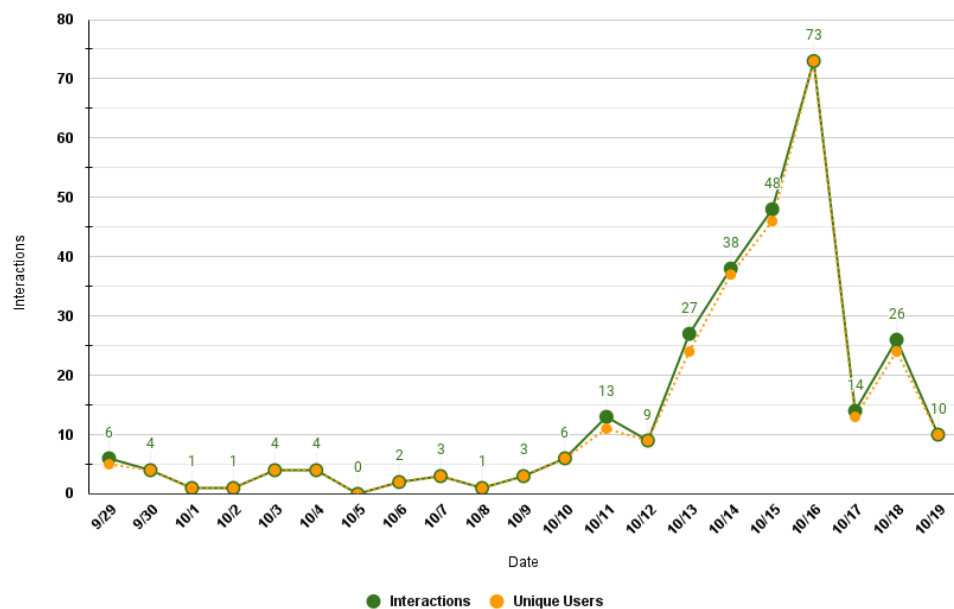
The chatbot use with different writing prompts for chemistry makes it possible to assess which aspects of the tool held students' interests the most. All analysis was carried out within an IRB-approved protocol, so only users who consented to have their actions within the chatbot aggregated are described further here. Anonymous user data collected was not used in this analysis since the chatbot was accessible for anyone visiting the webpage so people other than class participants may have accessed the tool. Over 87% of registered users of the chatbot agreed to have their interactions collected for analysis. Students who did not engage with the chatbot beyond the name collection were additionally eliminated from the analysis. A breakdown of several features of the usage by the sample of consenting participants is summarized in Table 1.

210 **Table 1:** Numbers for recorded users, interaction characteristics, chemistry topics and exploration characteristics from the implementation of the chatbot in a general chemistry course in Fall 2021.

Chatbot Users		Unique Users	Repeat Users	Total Interactions
		232	55	293
Interaction Specifics		Average Time	Average Steps	Average Actions
		4.1 minutes	14.5	7
Topics	None	Water footprint	Carbon footprint	Embodied Carbon
	56	115	79	17
Exploration Guide	Explore Chem Idea	FAQs	Sustainability	Have an Idea?
	63 Yes 230 No	54 Yes 239 No	171 Yes 122 No	58 Yes 77 No

Several observations in Table 1 merit specific notice. Over 41% percent of interactions featured a student who came back to the chat more than once (24.2% of users). Of the different modules available in the chatbot, sustainability drew larger numbers with 58.4% interactions activating one of the many avenues to explore that module. Students explored water or carbon footprint modules more than embodied carbon (39.2, 27.0, 5.8 percent of interactions, respectively) as the topic of interest. Students also were less inclined to visit modules in the chatbot on how to incorporate chemistry in their paper (21.5% did so). A more introductory engagement section, “Have an idea?” part of the chatbot, was used in 135 interactions (46%) of the interactions. This section of the decision tree was designed to aid student exploration dependent on how much of an initial idea a student had about approaching the paper. For this section, 43% indicated they had an idea for the paper and 57% indicated they needed inspiration from prompted topics from chatbot to explore. Many students followed the guidance of the chatbot’s prompts and choice; however, 19.8% (58) of interactions included direct student input that connected to trigger phrases learned by the chatbot to steer to another area that students were interested in gathering information.

On average, a chatbot interaction lasted approximately four minutes and explored seven intents. The chatbot was released to the students for a period of 21 days, and as seen in Figure 3, the bulk of the chatbot use was closer to the deadline of the written assignment, including peak usage on the weekend before the due date. When breaking down the times students interacted with the chatbot, 65.5% of interactions were done during the weekday versus 34.5% of interactions during the weekend.



235 **Figure 3:** A scatterplot of recorded chatbot interactions (green) and unique users (orange) over the course of the 20 days that the chatbot was released for student use. The last day depicted was the deadline for the writing assignment the chatbot was intended to provide aid for.

In total, the implementation of the chatbot in the chemistry classroom had a large reach with over
240 78% of students using the curated chatbot as built. There were 58 interactions (19.8%) that asked the
chatbot a question outside of its capability. From the perspective of the developers, there were learning
opportunities associated with the live implementation (Supporting Information – Item 3).

Importantly, this class-based scale of the implementation provided information about students’
perceptions of the range of the chatbot’s capabilities. Some participants clearly were more accustomed
245 to broad search engine interactions with web-based content. In cases where a student asked a very
specific and narrow question, as would be common with an internet search engine, a strong possibility
existed that this curated chatbot would be unable to address it. In some cases, the chatbot would turn
students toward information the chatbot did have built in, which could be perceived as an undesired
result. Thus, from an instructional perspective, it is important to provide students with guidelines
250 about strengths and limitations of using an instructor-curated virtual assistant relative to broad-
based search engine approaches (Supporting Information – Item 4).

CONCLUSION

The emergence of large-language model (LLM) resources such as ChatGPT, has brought significant
attention to the qualities of that form of virtual assistant in terms of writing assignments in
255 education.^{28–31} Although there are many different potential approaches to using such generative tools,
it is also important to recognize that curated chatbots, with intentional design parameters that frame a
particular educational use, represent an additional way to provide high value information to students.
The intent of such curated tools is not to provide example written responses, which has produced
concerns about the potential for students to submit assignments written by the LLM tools^{27–29,31,32,46}.
260 Rather, an instructor-constructed chatbot provides an interactive corpus for exploration targeted at
student understanding of the topic prior to the effort of creating an essay for a writing assignment. The
interactivity was designed to mimic conversational interactions, which is particularly helpful in large
enrollment courses⁴⁷. Including the pilot implementation, the curated chatbot had been featured in
subsequent semesters of both first and second-semester general chemistry courses featuring
265 sustainability context topics, i.e., nanochemistry in consumer products and carbon capture. The
appeal of curated chatbots can extend to other subjects. One use case, applicable to any classroom

setting, is to program a chatbot that breaks down the syllabus into its component parts for students to reference in a more interactive manner.

Using a curated chatbot to reach students at scale in a large lecture classroom to assist with details about a writing assignment connecting chemistry to sustainability contexts is described in this report. The analysis of log files of the use of the chatbot from a large number of participants in the course, provides evidence of their interest in using a tool that was readily accessible and broadly curated on topics relevant to a writing assignment. Furthermore, evidence of the use of the chatbot has been observed with students listing it as a cited resource in many submitted papers. Additional student papers incorporated references from articles that were presented as answers to student queries in the chatbot. Anecdotally, because this style of writing assignment has been used for many years by the instructor, the chatbot's implementation appears to have a broad positive impact on the quality of student papers. By providing an interactive resource with starting information for students to learn from, they appear to be better able to craft written work connecting chemistry in context.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI:

10.1021/acs.jchemed.XXXXXXX. [ACS will fill this in] Example brief descriptions with file formats indicated are shown below; customize for your material.

Item 1- Assignment Parameters

Item 2 – Chatbot Navigation

Item 3 – Curated Chatbot Development Notes

Item 4 – Curated Content Guidelines For Students

AUTHOR INFORMATION

Corresponding Author

*E-mail: taholme@iastate.edu

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