Developing Augmented Reality Mobile App for Learning Nucleophilic Substitution Reaction Mechanisms in Organic Chemistry: User Perception and Experience

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Abstract. A prototype AR mobile app "Immersive Nucleophilic Substitution" (INS) has been developed to assist students in understanding the concept of unimolecular nucleophilic substitution (S_N1) and bimolecular nucleophilic substitution (S_N2) reaction mechanisms. This study aims to examine the perception and user experience of the INS app among the university Foundation in Science students. An online questionnaire with a 7-point Likert scale was used to measure the perceptions towards the AR from the aspects of *performance*, *effort, social influence* and *motivation*, and the user experience in terms of *presence, usability, and flow.* Open-ended questions were included to further understand the participant's experience with the INS app. There were 29 responses collected. The overall perception of students was rather positive ($M = 5.00$, $SD = 1.00$). Students perceived the app as more beneficial to increase their learning productivity but less enjoyable and motivating. They felt the app provided sufficient realism, responded well to the students' actions and had a good-quality interface. However, it is somehow unnecessarily cumbersome, dull, and boring. The overall positive rating ($M = 5.55$, $SD = 1.33$) indicates the INS app was fairly well received by students and feasible to progress for the learning outcome evaluation.

Keywords: augmented reality · nucleophilic substitution reaction · chemistry · perception · user experience

1 Introduction

Augmented reality (AR) is a technology that superimposes computer-generated virtual content onto a real-world environment to provide a display of 3D objects that look real. Recently AR has risen as a potential tool to enhance spatial and visual skills, conceptual understanding, scientific inquiry learning, practical skills, and critical thinking and problem-solving skills in STEM education (Dunleavy et al., 2009). In chemistry and biochemistry education, AR has been developed to help students to visualize and

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manipulate various 3D structures of the molecules and improve the learning concept. Some examples include molecular geometry [1], the metabolic pathway from substrates to products [2], elements 4D [3], chirality-2 [4], DNA structure [5], the crystal structure of inorganic compounds [6], 3D molecular model based on crystallography data [7], and macromolecules and their potassium channel [8]. The application generally gained positive feedback. Students were motivated and had higher interest and enthusiasm to learn by using AR. They gained higher satisfaction compared to conventional learning through 2D visualization and were able to recall the information better. Ref [9] reported that AR intervention also helps special needs students to achieve better academics in the specific chemistry content.

Although the advances in AR technology have impacted various areas of chemistry, the application of AR in reaction mechanisms is less explored. Recently, ref [10] (2020) developed an AR mobile app (NuPOV) to study nucleophilic addition reactions. The app allows the users to simulate a nucleophilic attack for a nucleophilic addition reaction using their fingers, after fulfilling a set of specific reaction conditions stipulated by collision theory. The main focus was to assist students to understand the HOMO-LUMO interaction of nucleophiles with the electrophilic carbonyl groups during the reaction. To date, to our best knowledge, there has been no AR developed for the nucleophilic substitution reaction mechanism. In fact, learning nucleophilic substitution reactions is equally challenging as many of the reactions involve stereochemistry which adds spatial complexity to the context. In this project, we developed an AR mobile app prototype, "Immersive Nucleophilic Substitution" (INS), that can run on a mobile phone. INS app aims to improve the learning outcome of students on the topic of reaction mechanism, as well as enhance students' spatial and visual skills for future molecular studies. This paper reports the perception and user experience of the INS application among students in the Foundation in Science, University of Nottingham Malaysia.

2 Methodology

2.1 Content Design of INS Mobile App

The content of the INS app is aligned with the intended learning outcomes and assessment for the topic of haloalkane, Chemistry 2 module (SCIFF028), which is offered in the second semester of the school of Foundation in Science. Toward the end of the topic, students are expected to possess the visual-spatial thinking skills, and specific knowledge to perform the tasks of: (1) classifying primary, secondary, and tertiary haloalkane, (2) describing the characteristics of the two nucleophilic substitution pathways, namely unimolecular nucleophilic substitution (S_N1) and bimolecular nucleophilic substitution S_N2 (3) predicting which substitution reaction pathway a haloalkane would undergo at a given condition (4) deducing the reaction products with correct stereochemistry. Two types of nucleophilic substitution reaction mechanisms, which are S_N1 and S_N2, for primary, secondary, and tertiary haloalkanes with both symmetry and asymmetry structures were selected to develop. The app was designed to contain a variety of presentation modalities which include AR models, AR animations, graphs, and text.

2.2 Creation of 3D Models

Compounds MOL file was downloaded from Pubchem database. The MOL files were then imported into Unity and parsed to generate models. Spheres with proper size and color were generated to represent atoms and placed in the correct position. The relative atomic size was based on the Van der Waals radius scale (only for estimation purposes), whereas color was based on Corey-Pauling-Koltun (CPK) color scheme. Chemical bonds were represented by cylinders and colored according to the atoms they connected. The bond length was estimated according to the scaled empirical atomic radius [11]. A script was added to each atom containing extra information such as charge and location information. The script was then enabled to generate electron pairs for charged atoms. Electrons were made from small spheres positioned via simple handmade rules and kept as far apart as from each other, obeying valence shell electron pair repulsion (VSEPR) theory. The generated molecular shapes were then reordered in the unity hierarchy. A central atom was manually chosen, and the bonds and neighboring atoms (and electrons) were childed to it. The process was then repeated recursively for each of the neighboring atoms. A separate script was then enabled to find all atoms and their position on the screen (along with all other associated elements) and labeled them.

2.3 Creation of 3D Animations

A custom animator was made. It took n models with the same hierarchy structure to be used as a kind of animation step and $n + 1$ numbers. The numbers were timed to transition from one animation step to the next and timed to wait at the start and the end before (optionally) looping. The animator was then given a (t mod animation duration) time. The t value was used to lerp the local rotation of the atom around the bond which was nearest to the central atom. It also lerped the scale of all objects to allow atoms and/or bonds to fade/grow in/grow out/stretch for animation purposes. An animation series may consist of more than one individual animation running in parallel. A custom line renderer was used to draw the graph of energy level.

2.4 AR Software and Hardware

AR objects were made in Unity 3D. Vuforia was added for AR support. First, the texture generated by the phone camera was taken by Vuforia as input. The detection of the selected image target was then attempted. The detected virtual image target was placed where the actual image target was located, meaning at the position relative to the phone camera and virtual camera. As the 3D model was connected to the target, this also placed the 3D model in position. The generated apk file was then installed on the Android phone for the app application.

2.5 An Evaluation Survey

Research data were collected through a survey. The approval from the faculty's Research Ethics Committee was sorted to ensure that the ethical aspect of the participants was protected. The survey was administered to all Foundation in Science first-semester students

who have no background knowledge of chemical reaction mechanisms. Students were given the APK file to install on their mobile phones. This was made possible via Moodle announcement and shared by lecturers during the online classes. The participation was on a voluntary basis.

A three-part online questionnaire was used to evaluate how the INS app we developed impacted the learning experience of the participants. Part 1 measured perceptions towards the AR app using a questionnaire adapted from Udeozor et al. al [12]. The 11 items ($\alpha = .91$) were rephrased to reflect perception after the use of the app which included aspects of *performanc*e (2 items; $\alpha = .96$), *effort* (3 items; $\alpha = .95$), *social influence* (3 items; $\alpha = .90$) and *motivation* (3 items; $\alpha = .63$). In short, *Performance* indicates how far a person believes the AR app would allow him to perform a particular activity. *Effort* refers to the degree of ease associated with the AR app a person perceived. *Social Influence* explains how far a person perceives that people surrounding them thought that they should use the AR app. *Motivation* describes the degree of enjoyment when a person uses an AR app.

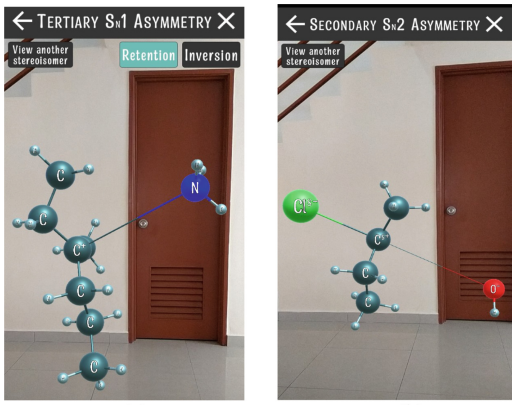
Part 2 examined the participants' evaluation of user experience with a questionnaire adapted from Rhiu et al. [13]. The questionnaire consisted of three dimensions: *presence* (15 items; $\alpha = .96$; which measured response to the action, realism, and quality of interface), *usability* (10 items; $\alpha = .77$) and *flow* (11 items; $\alpha = .92$). In short, *Presence* is defined as the user's sense of being there. *Usabilit*y measures how well the product is designed to achieve the goal. *Flow* measures how absorbed the user is with the app.

All items in Parts 1 and 2 were assessed on a 7-point Likert scale from 1 (strongly disagree) to 7 (strongly agree) and the quantitative data were analyzed using SPSS to obtain informative descriptive statistics. Finally, Part 3 consisted of three open-ended questions to help further understand the participant's experience with the AR app. These questions were adapted from Reeves et al. [14]. Participants were asked to provide three adjectives to describe their experience with the app, some things that they liked the most about the app, and some things they liked least.

3 Results and Discussion

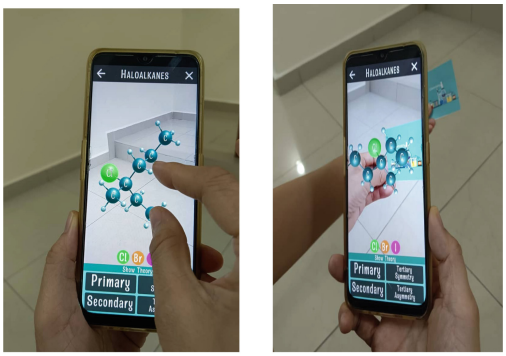
3.1 INS Mobile App

The INS app (https://tinyurl.com/2s3n5snf) we developed consists of 5 sections devoted to nucleophiles, halogens, haloalkanes, solvent medium, and mechanisms respectively. The theory for each section is provided in the drop-down list. Students can opt either to read the theory at the button or to escape the parts. Figure 1 shows examples of S_N1 and S_N2 mechanisms in the INS app. Students can interact and manipulate the models along the mechanism pathway using their fingers, which include inversion, enlargement, and rotation, as well as rotate the models in 3-axes by moving the printed marker to view the molecules from various angles (Fig. 2). INS provides not only the visual characteristics of the real shape of molecules through a 3D AR model but also the dynamic trajectories through 3D AR model animations. Students can view the spatial differences of various reaction mechanism pathways, the position of the nucleophilic attack on the electrophilic carbon, how the molecules interfere with each other, the formation and breaking of bonding, as well as the change of properties (e.g. lone pair electrons, charge, and energy



(a) (b)

Fig. 1. Examples of (a) S_N1 reaction and (b) S_N2 reaction



(a) (b)

Fig. 2. Students can (a) interact with the models using their fingers or (b) rotate the models in 3-axes using a printed marker

profile) throughout the reaction at an atomistic level. They can install and use this mobile app using a mobile phone or tablet and choose which reaction mechanisms they would like to interact and proceed with.

3.2 Students' Perception and User Experience

As a preliminary evaluation stage for the INS app, a survey was conducted among Foundation in Science students to investigate its perception and user experience. A total of 29 complete responses were obtained from the survey.

The overall perception of all students after using the INS app was rather positive ($M = 5.00$, $SD = 1.00$). Table 1 shows the perception of mean scores after using the app according to the measured constructs of *performance*, *effort*, *social influence*, and *motivation*. Students rated the app highest for being more beneficial to increase their learning productivity, however, students rated the app lowest for being enjoyable and

Table 1. Students' perception of the augmented reality app

Constructs	Mean	Standard Deviation
Performance	5.52	1.36
Effort	5.20	1.36
Social Influence	5.21	0.90
Motivation	4.23	1.28

motivating to use. The results were consistent with Aw *et al.* [10] who reported the NuPOV AR app they developed for electrophilic addition mechanism did not raise students' level of interest and did not motivate them to study tougher courses in organic chemistry, despite the app being useful. This could be because the reaction mechanism itself is a dull and tough subject that hardly attracts students' interest. Considering this, integrating auditory sensory elements such as audio narrative, background music, and sound play that respond to the interaction from users could be a viable way to make the INS app more attractive and expressive.

The INS app was rated as generally providing a relatively good user experience, especially in terms of *presence* ($M = 5.10$, $SD = 1.12$), indicating that the app provided sufficient realism, responded well to the students' actions, and has a good quality interface. This was further highlighted in the open-ended questions which will be discussed later in this section. Both usability ($M = 4.59$, $SD = .88$) and flow ($M = 4.73$, $SD = 1.09$), on the other hand, were rated slightly lower although still generally positive. The students did indicate that they thought the app was unnecessarily cumbersome ($M = 4.45$, $SD = 1.55$) and that they needed to learn a lot of things before they could get going with the app ($M = 4.17$, $SD = 1.89$).

Analysis of the open-ended questions uncovered some significant feedback that agrees with the quantitative findings. Students were generally more positive towards the INS app. Most of the students described the app as *educational, fun,* and *useful*, which agrees with the quantitative findings regarding students' perception of the app. However, there were students who also found the app "boring" which would explain why the rating for motivation was the lowest. This was indicated in the following student quote:

- The design is very plain, and simple, it doesn't give me any motivation to use the app.
- Students did mention that the INS app was *immersive*, *real,* and helps to *visualise.* The following student comments were not uncommon:
- The diagrams were very clear.
- Could see 3D shapes of molecules without going to YouTube.
- I can see the objects in 3D dimensions.

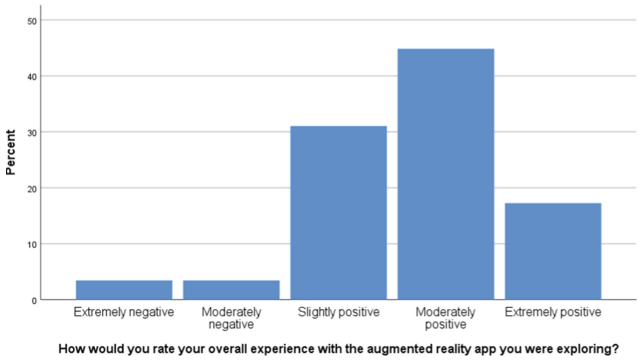


Fig. 3. Frequencies of students' perception of the AR app

- Enable 360-degree view of the molecules and easy adjustment of the sizes to view them.

Although enjoying the immersion ability of the INS app, students did mention that the app was *underdeveloped* and *glitchy* which agrees with the findings concerning *usability* and *flow*. The following student comments were some of the related comments:

- Diagrams were a bit laggy on zooming in and out and started out quite large, so I couldn't see the whole model at first glance.
- Limitations on the movement of the atoms and how disconnected it felt from the real world.
- The adjustment of the size of the molecules is not flexible enough.

Finally, when asked how they would rate the overall experience with the INS app they were exploring, the students' response was rather positive ($M = 5.55$, $SD = 1.33$; see Fig. 3 below for frequencies).

4 Conclusions

In this project, we have developed an AR mobile app (INS) in which students can interact with 3D models and 3D animations with their fingers on a mobile phone or tablet. The INS app is expected to provide visual representations and spatial cues to enhance students' understanding of the concept of S_N1 and S_N2 mechanisms, as well as the stereochemistry involved. Despite there being some room for improvement, the prototype received relatively positive responses on the perception and user experience of students. Future studies will focus on how well students learn using the INS AR app we developed compared to the conventional method with a validated assessment tool in a classroom setting.

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