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The Effects of PhET Simulations on Students' Experienced Immersion and Understanding of Molecule Shapes

Leonardo M. Francisco Jr.[1], Florence Garcia[2], Dolores C. Mirabueno[3]
[1]De La Salle University, Manila, Philippines - 1004
[2]St. James Academy, Science Department, Manila, Philippines - 1470
[3]De La Salle-College of Saint Benilde, Antipolo City, Philippines - 1870
leonardo_m_franciscojr@dlsu.edu.ph, science_fgarcia@stjamesacademy.edu.ph, dolores.mirabueno@antipolo.benilde.edu.ph

Abstract— *This action research makes use of PhET simulations as a learning intervention to explore its effect on students' experienced immersion and understanding of the concept of molecular geometry, while also looking into the correlation of the two variables. It is a quasi-experimental study that makes use of the PDSA model. The participants are 66 intact grade 11 students from a private school in Metro Manila. The instruments used to gather quantitative data are pre and post concept tests and survey about immersion levels, while qualitative data were drawn from journal entries and FGD transcripts. The results suggest that PhET is an effective tool in enhancing students' conceptual understanding of complex lessons in chemistry, while also providing high engagement through its interactivity and ease of use. However, it may not be sufficient in providing total immersive experiences for learners.*

Keywords— *PhET simulations, experienced immersion, conceptual understanding, moleculular geometry, learning gain.*

I. PLAN

Defining the System

There is a consistent need to improve the quality of education, especially in the face of rapid globalization. In the Philippines, the necessity to enhance science education has been a priority since the country lags behind other countries in terms of students' understanding of science concepts, as translated to reasoning and analytical skills (Sadera, Torres, and Rogayan, 2020). Such problems that plague science education in the country include lack of instructional materials, inadequate facilities for learning, insufficient teacher training, and lack of motivation and interest among learners (Kaptan and Timurlenk, 2012). Although there is a gap between public and private schools in terms of access to learning materials and facilities, difficulty in learning science still prevails due to its contents having intricate terminologies and very abstract concepts, making it grueling for some learners. This is no more apparent than the lessons tackled in chemistry, where abstract phenomena go against the learners' pre-instructional conceptions (Treagust, 2006). Hence, educators must employ innovative practices to help students understand very complex concepts, such as those under chemistry.

Assess Current Situation

The current state of technology opened the door to advances in visualization that allow interactions with complex phenomena that are not apparently observable, thereby supporting cognitive understanding (Evagorou, Erduran, and Mäntylä, 2015). Multimedia learning has been proven to be effective in conveying concepts to learners, while computer generated models of chemical structures have been confirmed to enhance comprehension among learners from primary to higher education (Ferk, Vrtacnik, Blejec, and Gril, 2003). The effectiveness of these media tools can be attributed to their ability to immerse learners through the stimulation of multiple senses, such as when a learner manipulates 3D objects with the use of visuals, touch, and sound. One of the leading computer-generated visuals that aide in learning chemistry is Physical Education Technology (PhET) simulations – a collection of computer interactive simulations designed for learning physics, chemistry, math, among others (Salame and Makki, 2021). Simulations in chemistry come in the form of computer-generated simulations of particles not seen by the naked eye, such as atoms and molecules (Beichumila, Bahati, and Kafanabo, 2022; Bhatti, Teevno, and Devi, 2021; Dunn and Ramnarain, 2020; Mallory, 2023; Mashami, Ahmadi, Kurniasih, and Khery, 2023; Nkemakolam, Chinelo, and Jane, 2018; Penn and Ramnarain, 2019; Sa'diyah and Lutfi, 2023; Sibinda and Shumba, 2022).

A meta-analysis conducted to see the trends in the use of simulations in teaching and learning chemistry revealed a movement in the adoption of the said technology, pointing to its effectiveness in helping students understand concepts that range from acid-base reactions, atomic structure, balancing of chemical equations, chemical bonding, to molecular geometry (Beichumila, Bahati, and Kafanabo, 2022; Bhatti, Teevno, and Devi, 2021; Dunn and Ramnarain, 2020; Mallory, 2023; Mashami, Ahmadi, Kurniasih, and Khery, 2023; Nkemakolam, Chinelo, and Jane, 2018; Penn and Ramnarain, 2019; Penn and Ramnarain, 2019; Sa'diyah and Lutfi, 2023; Sibinda and Shumba, 2022). These literatures proved a large effects size (1.28) for the use of simulations as learning intervention, with an equal positive outcome in engagement and motivation. Several literatures also mention "immersion" and "immersive technology" in discussing the effectiveness of the use of simulation in learning. However, there is no

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concrete exploration of the said construct in any of the literatures reviewed. Fig. 1 shows the comparison of the effects sizes of the nine (9) studies included in the meta-analysis with an overall effects size of 1.28, which means high gain. This suggests that the use of simulations in teaching has a very positive effect in the conceptual understanding of learners.

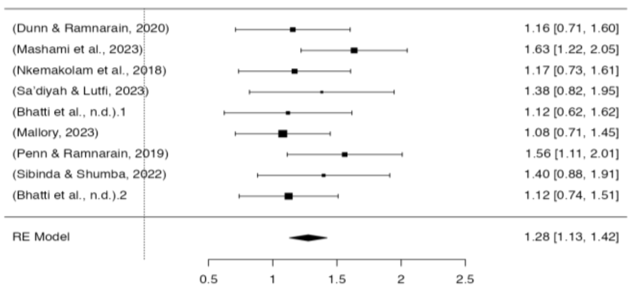

Fig. 1. Forest plot that shows the effects sizes of the 9 studies included in the meta-analysis and the overall effect size of 1.28.

According to Georgiou and Kyza (2017), immersion is a construct widely used in video games, but its actual presence in the use of immersive media tools in learning is poorly understood. Some researchers argued that immersion is not only experienced in the context of video games, but is a human state that could emerge in activities that are engaging or engrossing (Brooks, 2003; Weibel, Wissmath, and Mast, 2009; Witmer and Singer, 1998). Hence, entertainment and learning can depend on the degree of immersion the person experiences, or the degree to which they become engaged and engrossed by a multimedia application (Brooks, 2003; Cheng, She, and Annetta, 2015; Dede, 2009) posit that immersive can support science learning through a.) comprehension of complex scientific phenomena, b.) active learning, c.) and translation of learned skills into real-world applications.

Analyze Causes

Rogayan, Rafanan, and De Guzman (2021), mentioned that one of the main challenges of Science, Technology, Engineering, and Mathematics (STEM) learning is the level of difficulty, as seen in courses that are hard to comprehend. Among these courses is general chemistry – which deals with phenomena that occurs in the molecular levels – a very abstract concept that can be hard to connect with learners, especially if insufficient learning materials are used (Rahmawati, Andanswari, Ridwan, Gillies, and Taylore, 2020). Particularly, learners are challenged to comprehend lessons in Valance Shell Electron Pair Repulsion (VSEPR) theory and molecular geometry because traditional static visual aids do not fully demonstrate these phenomena (Stiawan, Basuki, Liliasari, and Rohman, 2022).

The purpose of this action research is to address the difficulties of students when it comes to learning the lessons about VSEPR. Baseline data, which are based on past test scores and interviews, revealed that students do not fully comprehend how molecular shapes are influenced by forces of repulsion among the paired and unpaired electrons. Hence, the researchers investigate the effects of using PhET simulations on students' understanding of the concept of VSEPR, and their experienced immersion in the use of the simulation.

This action research aims to answer the following research questions:

1. What are the students' conceptions of molecular geometry before and after the use of PhET simulation?
2. How do the gains in test scores reflect the effectiveness of the use of PhET simulations?
3. What are the students' levels of immersion when they use PhET simulations?
4. How do immersion levels correlate to students' learning gains?

II. DO

Research Design

This action research employs the Plan-Do-Study-Action (PDSA) method that utilized a quasi-experimental design. It uses a mixed-methods approach that employed a one-group pretest-posttest procedure, and a sequential explanatory approach of quantitative and qualitative data from questionnaires, focus group discussions (FGD), and journal entries. The pretest and posttest, implemented before and after the use of PhET simulations, provided the data to gauge the effectiveness of the intervention, while the survey forms, FGD, and journal entries are used to explore the students' experienced immersion. Fig. 2 shows the framework of the study.

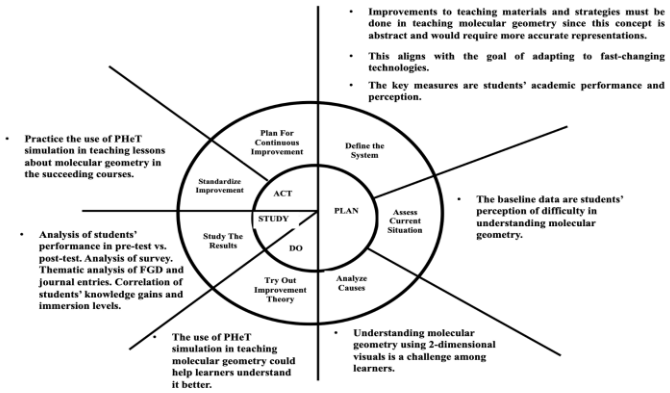

Fig. 2. Framework of the study in PDSA format

Research Participants

The participants were an intact group of Grade 11 students studying in a private school in Metro Manila, Philippines. All participants were enrolled in a STEM strand, with a total number of n = 66 – a combined two sections taking up general chemistry I for the school year 2023 to 2024. Participants for the FGD sessions (n = 12) were selected from the group based on their performance on the posttest, resulting to a combination of high achievers (n = 6) and low achievers (n = 6). Parents' consent was required for all participants before the implementation of the study.

Research Instrument

To gauge the students' knowledge about VSEPR and molecule shapes, a concept test was adopted from the works of

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Stiawan, Basuki, Liliasari, and Rohman (2022). It is a 25-item multiple choice test that covers the concepts of lone pair and bonding pair electrons, electron repulsion, molecule geometry, and polarity based on molecule shape. The concept test was evaluated by experts and experienced teachers of general chemistry to check for content validity and alignment with the curriculum. In exploring the students' level of immersion, a survey questionnaire developed by Georgiou and Kyza (2017). This instrument known as Augmented Reality Immersion (ARI) questionnaire, is a 21-item 7-point Likert scale survey that measures the students' experienced immersion levels. In addition, validated journal entry prompts and FGD questions were also developed by the researchers to parallel the ARI questionnaire in the collection of qualitative data. Lesson plans reflecting the intervention were also prepared by the researchers and were validated by the experts.

Implementation and Data Collection

The implementation and data gathering ran for 5 days. It began with the orientation of the research to the participants on the use of PhET simulations in learning the lessons about VSEPR and molecule shapes, before they answered the pretest using pen and paper. The learning intervention occurred for 3 days as summarized in Table 1.

TABLE 1. Summary of intervention showing duration, lesson, and learning objectives, and learning activities.

Duration	Lesson	Learning Objectives	Learning Activities
Day 1 (50 minutes)	Valence Shell Electron Pair Repulsion (VSEPR)	1. Describe the concept of VSEPR; 2. apply the AXE method to assign bonding pairs and lone pairs; and 3. construct correct 3D molecular models based on a given chemical formula or Lewis's structure.	• Motivation using short videos. • Guided inquiry through manipulation of molecule to learn VSEPR. • Gamified activity in building molecules based on formula type. • Assessment and journaling
Day 2 (50 minutes)	Molecule Shapes and Bond Angles	1. Identify the molecular geometry of simple compounds; 2. describe the bond angles of certain molecular geometries	• Motivation using short video. • Gamified activity – molecular geometry challenge. • Guided inquiry – observing bond angles. • Assessment and journaling
Day 3 (50 minutes)	Polarity	1. Describe the concept of polarity; 2. determine a compound's polarity based on electronegativity difference; 3. identify a compound's polarity by observing its 3D molecule.	• Motivation using demonstration – oil and water mixture. • Video that discusses about polarity. • Assembling molecule shapes and determining its polarity.

The PhET simulations for molecule shapes were accessed by the students using individual hand-held tablets, while the links and assessments were also accomplished in the same device through the Learning Management System (LMS). The ARI questionnaire was given to the students as a Google form which they needed to accomplish in answering the assessment on the 4th day. The posttest was given on the 5th day of implementation as a summative assessment. Based on the results, 12 students were selected to participate in the FGD on the same day.

III. Study

Students' Conceptions of Molecular Geometry

Fig. 3 shows the comparison of pretest and posttest of the 66 participants. The pretest has a mean of 8.12 while the posttest has a mean of 15.76, an increase of almost two folds after the use of PhET simulations. The lowest and highest scores for pretest are 3 and 14, respectively. This suggests that students lack knowledge of the concepts of VSEPR, molecule shapes, and polarity. On the other hand, the posttest has the lowest and highest scores of 6 and 24, respectively, suggesting a gain of knowledge after the intervention.

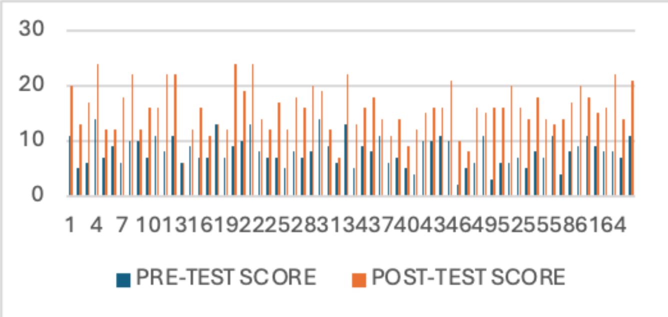

Fig. 3. The comparison of the pre-test and post-test

Paired t-test was used to analyze the difference between the pretest and posttest scores. The result of the analysis, as shown in Table 2, revealed a p value of less than 0.01 ($p<0.01$), which means that there is significant difference in the students' knowledge before and after using PhET simulation.

TABLE 2. Paired Samples of t-test of Pretest and Posttest.

			statistic	df	p
Pretest	Posttest	Student's t	-17.4	65.0	< .001

Note. H_a $\mu_{\text{Measure 1 - Measure 2}} \neq 0$

Students' Score Gains

The gain scores of each student was determined using Hake's formula, where the difference between pretest and posttest were divided by the total test score minus the pretest score (Azita Seyed Fadaei, 2019). It can be seen in Fig. 4, wherein the students are grouped according to their normalized gains. Among the students, 18% had high **g** – suggesting a significant improvement in learning, while 56% of the participants medium **g** – indicating a moderate improvement in their learning, and 26% had low **g** – a relatively low improvement in understanding.

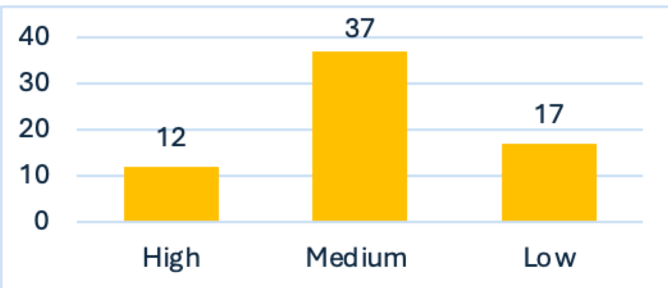

Fig. 4. The number of students with high, medium, and low N-gains.

The computed averaged normalized gain (N-gain) is 0.45, which is classified as medium g. Despite this, Hake (1998) posits that medium g normally result in courses with active-engagement instruction, compared to pure lecture courses that normally result in low g. Therefore, we can conclude that the use of PhET simulation has advantage over traditional classroom practices as reflected by the students' score gains.

Students' Immersion Levels

Fig. 5 shows the mean for each level of immersion. Georgiou and Kyza (2017) explained in their development of the ARI questionnaire that immersion can be organized into three levels, namely "engagement", "engrossment", and "total immersion". Further, engagement can be broken into the constructs of attraction, time investment, and usability.

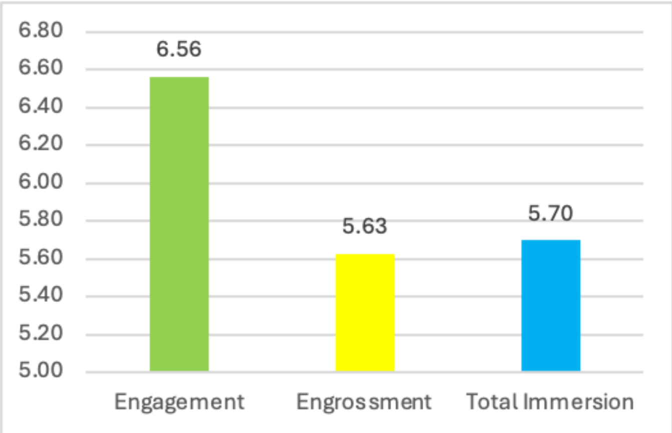

Fig. 5. Mean values for engagement, engrossment, and total immersion.

Meanwhile, engrossment is formed by emotional attachment and decreased perception of the natural environment. Finally, total immersion consists of presence and empathy. The results suggest that the use of PhET simulation result to very high engagement among students, but it was not as effective in bringing the students' level of immersion to engrossment and total immersion.

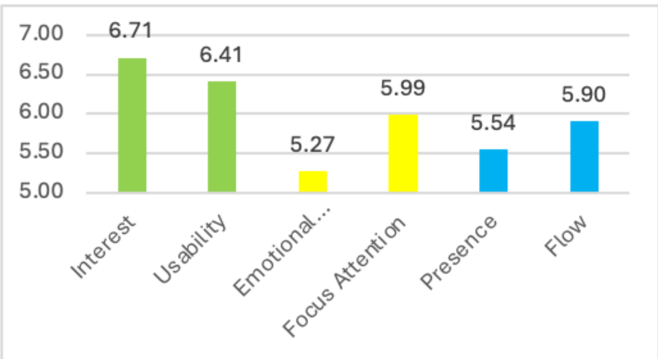

Fig. 6. Mean values for the components of immersion.

Exploration of the components of immersion, as seen in Fig. 6, shows that the students gave high ratings to interest and usability when using PhET simulations, while they gave low ratings to components under engrossment and total immersion, particularly emotional attachment and presence. Georgiou and Kyza (2017) further explains that high ratings in the components of engagement suggests that students developed high interest, with willingness to spend time completing the tasks, and perceiving the learning material as a very useful.

To support the results of the survey, data from journal entries and FGD sessions were thematically analyzed using the method proposed by Braun and Clarke (2006) as a strategy to explain the students' ratings. Fig. 7 shows the codes derived from the analysis.

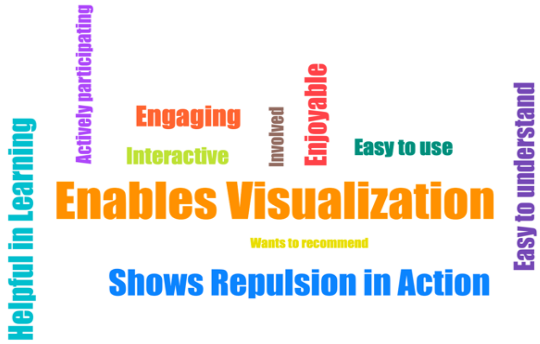

Fig. 7. The codes derived from the journal entries and FGD transcripts.

The most frequently mentioned by the students during the journal entries and FGD are the words related to PhET's ability to provide interactive visualization of the 3D molecules. The students also gave emphasis on high engagement, enjoyment, and usefulness of the use of PhET.

Relating the students' answers to their ratings in ARI result to several interesting themes.

Theme 1: The PhET simulation results to high engagement due to its novelty, ease of use, and perceived enjoyment and usefulness.

The use of PhET provided new experiences for students because it allowed them to visualize and interact with abstract objects such as molecules. They pointed that simulation does not require any learning curves and has features that are very intuitive. As one student wrote in the journal entry:

> *"I was enjoying moving the molecules around. I was curious about how to understand this when I already had learned how to use Phet simulations. It was easy to use and convenient. I was able to see how to visualize molecules in 3D." - Journal Entry Transcript - BJM, Pos. 118*

This reflection agrees with the high ratings given by the students to items under engagement.

Item no.	Statement	Mean	SD
1	It was easy for me to use the simulation	6.83	0.48
2	I wanted to spend the time to complete the activity successfully	6.66	0.61
4	I liked the activity because it was new	6.71	0.70
5	I found the AR application confusing	1.90	1.31

Theme 2: The learners find PhET simulations lacking when it comes to game-like experience.

Although the students find PhET simulation engaging and very helpful in understanding molecule shapes, they find it deficient when it comes to features that could make it more game-like. As digital natives, the students have high expectations as to how a simulation could be more exciting to use, showing tendencies to compare PhET simulation to interactive games they play in their devices. As some students mentioned in FGD:

> *"Kasi po wala pa po masyadong puwede explore. Para pong may kulang pa po na something to add* (because there are no other features to explore, and I think there are still something to add)." - *FGD transcript - PhET simulation, Pos. 156*

> *"Meron kaming nilalarong app nila collen it's like atoms and when we press it, it will spread out (*me and collen have an apps that we play, it's like atoms and when we press it, it will spread out*)." - FGD transcript - PhET simulation, Pos. 82*

These remarks reflect the ratings that the students gave to a question under engrossment.

Item no.	Statement	Mean	SD
17	I often felt suspense by the activity	3.71	1.93

Theme 3: Most students did not reach total immersion because the regular classroom interactions prevented this.

The ARI questionnaire was designed by the authors for interventions that make use of location-based AR applications, where students are given the reign to explore their surroundings, while being away from the normal class routines. The analysis revealed that some students failed to experience total immersion because their attention was split between the simulation and the stimuli in their surroundings. As one student mentioned in FGD:

> *"Ayun po pag may katabi po akong parang... mag tatanong during our discussion mag tatanong na parang tama ba? to check if their answer is correct* (whenever my seatmate will ask me during discussion if their answer is correct to check and confirm if their answer is really correct)*." -FGD transcript - PhET simulation, Pos. 65*

This statement agrees with the rating of the students they gave to one of the components of total immersion.

Item no.	Statement	Mean	SD
21	I so was involved, that I felt that my actions could affect the activity	5.34	1.69

Correlation Between Immersion Levels and Student Performance

TABLE 3. Multiple regression for components of immersion and student performance

Predictor	Estimate	SE	t	p
Intercept	3.615	7.175	0.504	0.616
Engagement	2.337	1.199	1.950	0.056
Engrossment	-0.346	1.071	-0.323	0.748
Total Immersion	-0.189	0.855	-0.221	0.826

Table 3 shows multiple linear regression involving the components of immersion as independent variables, while the student post-test score as the independent variable. It has an R2 value of 0.25, which means that 25% of the variance of the dependent variable is explained by the independent variables. Although none of the components of immersion had a p value lower than 0.05, it means that engagement has a near value of 0.056, suggesting that it correlates more compared to the other components of immersion.

IV. ACT

Pedagogical Implications

The results of this study imply that the use of PhET simulations in learning abstract concepts of VSEPR and molecular geometry can be beneficial in improving the students' understanding of the concept. The ARI questionnaire, together with the data from journal entries and FGD point to the high engagement of learners in the use of PhET simulations, but it also revealed that its insufficient in providing a total immersive experience for learners.

Recommendations for the Next Cycle

The use of other immersive multimedia learning materials should be used in combination with other instruments that explore the constructs of immersion.

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