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Effects of Computer Simulations, Attitudes Towards Chemistry and Prior Knowledge on Students' Academic Achievement in Chemistry

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Abstract. Improving academic achievement and students' attitudes towards chemistry are among the important goals of science education. This study aimed to determine the influence of computer simulations on students' attitudes and examine the predictive effects of the attitudes, students' prior conceptual knowledge and computer simulations on their academic achievement after being taught chemical kinetics. The mixed-method study was based on the constructivist learning theory with a quasi-experimental design to collect quantitative data and semi-structured interviews to collect qualitative data. An experimental group of 53 grade 12 students was taught using simulations, and a control group of 65 students was taught using the conventional approach at two secondary schools in Limpopo Province, South Africa. A questionnaire and an achievement test were used to collect the data, which were analysed using IBM SPSS Statistics version 28. An independent samples t-test showed that there was a statistically significant difference in the students' attitudes after instruction (t = 5.682, p < .05, d = 0.48) in favour of the experimental group. A stepwise multiple linear regression analysis revealed that attitude, students' prior conceptual knowledge and computer simulation instruction were significant predictors of academic achievement (prior knowledge: β = 0.49, t = 6.712, p < .05, attitude: β = 0.18, t = 2.248, p < 0.05, and instructional method: β = 0.40, t = 4.886, p < .05). Students with more positive attitudes, higher prior knowledge and who learnt using computer simulations had greater academic achievement. These findings have implications for practising teachers, as using computer simulations in teaching chemistry can result in improved academic achievement and attitudes towards chemistry.

Keywords: academic achievement; attitudes; chemical kinetics; chemistry; computer simulations; prior knowledge

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1. Introduction

Students' academic achievement is an essential indicator of the quality and effectiveness of instruction (Koçak et al., 2021). Thus, attempts to improve teaching effectiveness are critical to enhancing students' academic achievement in science education (Mikeska et al., 2017). Many countries invest financial and human resources into improving the quality of science instruction, as science subjects are closely associated with economic development (Mao et al., 2021). Improving the academic achievement and attitudes of students in sciences increases the chances of them pursuing careers in science and technology-related fields (Bellová et al., 2023), which contribute towards the technological development of a country.

Recent research indicates great concern about how academic achievement in science subjects such as chemistry, biology and physics could be improved (Sibomana et al., 2021; Sugano & Nabua, 2020). Students' academic achievement in science shows the effectiveness of instructional strategies (Nabizadeh et al., 2019). Academic achievement in chemistry is a multivariate construct, as it can be assessed through various indicators (Vilia et al., 2017). It is influenced by cognitive and non-cognitive variables such as prior knowledge, cognitive abilities, motivation, intelligence, interest, attitude and learning strategies (Nabizadeh et al., 2019; Xu et al., 2013). Affective factors such as self-efficacy and attitude impact students' feelings when learning chemistry (Flaherty, 2020) and some studies have shown that improving these affective factors can enhance academic achievement.

Numerous previous studies have explored the relationship between students' academic achievement in chemistry and psychological constructs such as attitude, metacognition and motivation (Flaherty, 2020; Samuel & Okonkwo, 2021; Vilia & Candeias, 2020). However, these studies have produced mixed results, with some confirming that improving these psychological factors results in increased chemistry achievement and other studies suggesting that improving the psychological factors had no effect (Chan & Bauer, 2015). Other studies have also examined the relationship between teaching methods and academic achievement, indicating that improving teaching methods leads to raised academic outcomes (Savelsbergh et al., 2016). Nevertheless, few studies have examined the influence of prior knowledge on academic achievement in Chemistry at the secondary school level (Seery, 2009). No studies in the reviewed literature were found to have investigated the effects of all three variables - prior knowledge, attitude, and instructional method- on academic performance. This study attempts to close the knowledge gap to investigate which of these constructs has a greater influence on academic achievement. Identifying the most significant variables may help teachers place more emphasis on them so as to improve academic achievement. This is the gap that the present study attempted to fill and which was carried out using the lens of the constructivist learning theory and information processing model.

2. Theoretical Framework

The basic premise of constructivist learning theory is that knowledge is not simply transmitted from teacher to learner; instead, students construct their own understanding (Alanazi, 2016). Cognitive constructivism postulates that learning occurs through the active construction of knowledge when students interact with their environment based on what they already know (Alanazi, 2016). In Piaget's theory, assimilation occurs if students integrate new knowledge into schemas, while accommodation involves modifying existing schemas (Bormanaki & Khoshhal, 2017). Students possessing prior knowledge of a concept are likely to be able to assimilate new knowledge successfully.

Vygotsky's sociocultural theory, on the other hand, postulates that learning occurs when the learner interacts with more knowledgeable persons (Vygotsky, 2011). When using computer simulations in instruction, the teacher provides support and guidance within the student's zone of proximal development (ZPD) (Figure 1). This support fades away as the learner gains more competence, and, at that point, the student can explore the experiments within the simulation without assistance. Scaffolding within the ZPD has been interpreted to refer to the support that the student receives from the more knowledgeable person and the mediating tools such as computer simulations (Fraser et al., 2015).

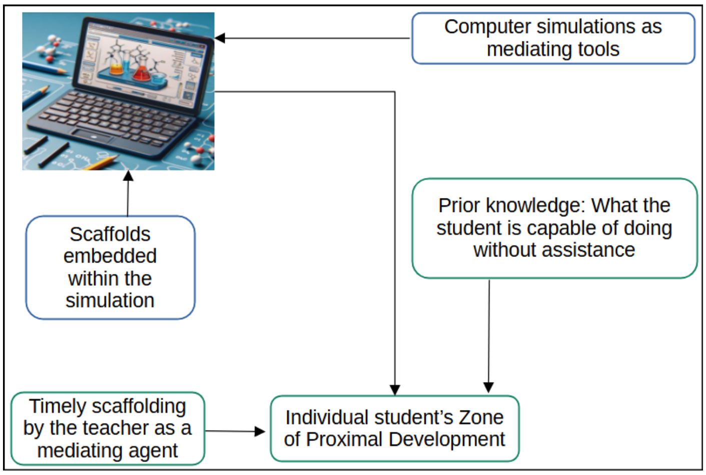

Figure 1: ZPD with the teacher and computer simulations as mediating agents

The information processing model (IPM) (Figure 2) is used in this study to understand how students can cope with the information within the computer simulation and how the teacher can assist in this process. IPM emphasises three constructs - perception, working memory and long-term memory (Johnstone et al., 1994).

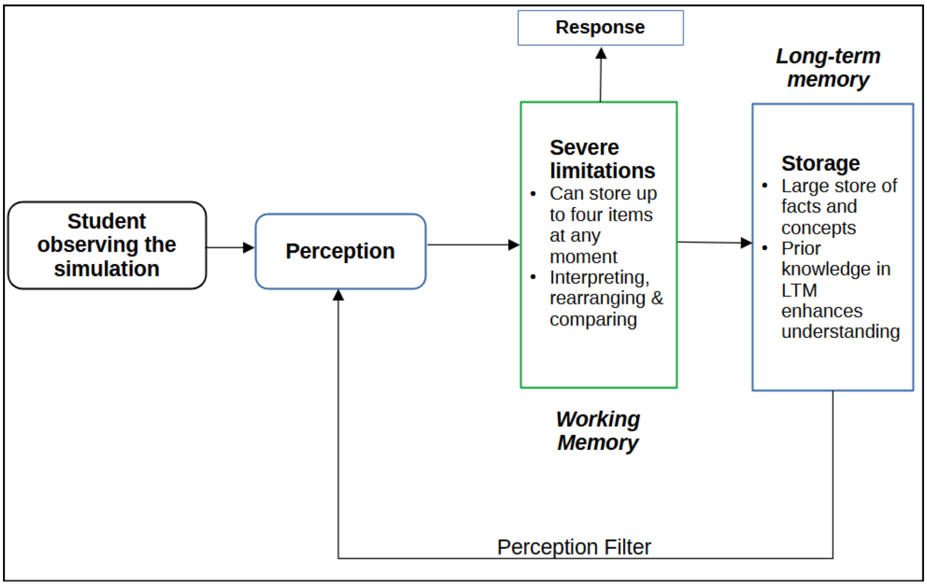

Figure 2: Information processing model adapted from Johnstone et al. (1994)

2.1 Perception

When the simulation is introduced to students, there is a lot of information within the simulation, all of which appears to be important. However, the learner lacks knowledge in long-term memory to differentiate 'noise' from 'signal' (Johnstone et al., 1994); therefore, the teacher's role is to direct students to important aspects of the simulation.

2.2 Working Memory

Working memory is the space in which information from the simulations interacts with information from long-term memory, resulting in understanding (Johnstone et al., 1994). It plays a role in holding and manipulating information in cognition, such as the effect of temperature, surface area or concentration on the reaction rate when learning chemical kinetics (Figure 2). However, it has severe limitations in capacity and can hold only up to four items at any moment (Bouchacourt & Buschman, 2019). It is critical, then, that the overloading of the students' memory when using simulations is prevented by guiding them to the essential aspects of the simulations.

2.3 Long-Term Memory

Long-term memory is a large store of concepts, facts, and ideas in the learner's mind (Johnstone et al., 1994). In the context of this study, long-term memory relates to the ability of students to retain and recall information on reaction kinetics over an extended period, such as days or weeks. Recalling and explaining concepts such as calculating reaction rates, explaining the effects of catalysts on reaction rates, and applying this information to novel situations demonstrate conceptual understanding and storage of the information in long-term memory (Jere & Mpeta, 2024). If the learner has prior knowledge of the concepts in the simulation, it enhances his/her understanding and interpretation of the information from the simulation (Figure 2).

The information processing model was also used to understand how students' attitudes form and change. Students use information stored in memory about an attitude object when forming an attitude towards that object. Attitudes can be formed about an attitude object even if the information was acquired in as little as a few minutes previously (Jacoby et al., 2002). Students form favourable attitudes when the attitude object is associated with positive characteristics and unfavourable attitudes when it is associated with negative characteristics (Maio et al., 2018). In this regard, both affect and belief about an attitude object are critical in the determination of the students' attitudes. The students' evaluation of an attitude object (in this case - the instructional approach) is a result of their readily accessible beliefs regarding the attitude object (Ajzen, 2012). When an instructional approach to learning chemistry is associated with positive characteristics, such as enhancing conceptual understanding, such a teaching approach would likely lead to the formation of positive attitudes.

3. Literature Review

Computer simulations are computer programs that contain models of natural or artificial systems used in learning chemistry (Abar et al., 2017). When used for teaching, they enable students to engage in scientific inquiry, which enhances learning through the active construction of knowledge (Çelik, 2022). In inquiry activities, students design experiments, test hypotheses, collect and analyse data and draw conclusions (Pedaste et al., 2015). This develops their science process skills (Çelik, 2022). Computer simulations' dynamic and interactive nature allows students to engage in these exploratory scientific enquiry activities. In conventional instruction, on the other hand, students are passive, and learning occurs by rote memorisation of information provided by the teacher (Golder, 2018) or reading from textbooks. Examples of conventional instruction include lecturing and direct instruction. This approach is not supported by constructivist learning theory and is ineffective in meaningfully learning complex and abstract concepts in chemistry.

Learning using computer simulations can increase learning outcomes in chemistry, potentially improving students' conceptual understanding (Plass et al., 2012). However, some students may find it difficult to understand chemistry because of the abstract nature of chemical concepts. As such, simulations provide a dynamic visualisation of chemical phenomena of atoms, molecules and ions at the sub-micro level, thereby simplifying abstract chemical concepts (Herga et al., 2016). When learning using computer simulations, students actively construct knowledge as they interact with these simulations with the teacher facilitating learning by coaching, guiding and providing support when needed (Golder, 2018). Inquiry activities such as the Predict-Observe-Explain strategy and collaboration among students when learning using computer simulations provide an engaging classroom environment that improves meaningful learning and can improve academic performance (Kearney, 2004).

Using computer simulations in teaching students will likely influence their academic success and other affective variables such as interest and attitude. An attitude is an individual's predisposition to like or dislike an attitude object, which in this study is the instructional approach used by the teacher (Krosnick et al., 2018). In this study, the attitude object refers to the chemistry lessons taught using the conventional approach or computer simulations supported by the Predict-Observe-Explain strategy. Students' attitudes towards these lessons were understood to be the attitude of students towards chemistry. Compared to conventional instruction, which is teacher-centred and uses the lecture method, research on the effects of some novel instructional approaches on students' attitudes towards chemistry has produced inconclusive results (Chan & Bauer, 2015; Younis, 2017; Zudonu & Njoku, 2018).

Younis (2017) investigated the effect of scientific enquiry simulations on students' attitudes towards chemistry and found that the experimental group taught using simulations had improved attitudes towards chemistry after instruction compared to the control group. Similarly, Zudonu and Njoku (2018) studied the effects of virtual laboratory instruction on academic achievement and students' attitudes towards chemistry and found that virtual laboratory instruction positively affected students' achievements and attitudes compared to conventional instruction. Chan and Bauer (2015) investigated exam achievement and affective characteristics of undergraduate students in chemistry using an experimental design, with the experimental group receiving peer-led team learning while the control group did not receive this treatment. They found no significant differences in achievement, attitude, or self-concept between students who participated in peer-led team learning and the control group. The instructional approach was found not to affect the students' attitudes.

The researchers also investigated how teaching chemical kinetics using computer simulations affects students' academic achievement compared to conventional instruction. A corpus of research has demonstrated that technology-based instruction, such as computer simulations, results in improved student academic achievement compared to conventional teaching approaches (Savelsbergh et al., 2016; Schroeder et al., 2007; Sugano & Nabua, 2020). While these studies all suggest that using technology in learning science improves academic achievement, they show differences in the effect sizes of the interventions.

While numerous studies have explored the effects of various innovative teaching approaches on academic achievement, there is still a need to examine the relationship between attitude and academic achievement (Kahveci, 2015; Sugano & Nabua, 2020; Xu et al., 2013). For example, it was demonstrated that success in and achievement of previous chemistry courses in middle school affected high school students' intellectual and emotional attitudes towards chemistry (Kahveci, 2015). Similarly, Xu et al. (2013) investigated mathematics ability, prior conceptual knowledge and attitude towards chemistry's effect on academic achievement among undergraduate students and found that each of the three variables significantly affects student achievement. These studies demonstrate that academic achievement in chemistry can be improved by fostering students' positive attitudes towards chemistry.

Two teaching strategies were compared in this study. The experimental group was taught using computer simulations supported by the Predict-Observe-Explain (POE) strategy (Gunstone & White, 1981) and the control group was taught using the conventional approach. POE represents a dynamic learning strategy that starts with students using their prior knowledge to predict the results of a simulation task. They then engage in an experiment using digital simulation to investigate the effects of some factors on reaction rates. Finally, students compare their initial predictions with their observations. Should there be any differences, they work on understanding and explaining these discrepancies to reconcile any conflict (Jere & Mpeta, 2024).

In contrast, the conventional method is a teacher-centred approach characterised by the teacher delivering lectures and explaining scientific concepts, with students passively listening and jotting notes (Wang et al., 2022). In this study, the control group's instruction did not incorporate simulations; instead, the teacher explained all concepts in chemical kinetics and assigned exercises for to be done at home to enhance students' comprehension. The only difference between the experimental and control groups within the study was the instructional methodology employed.

4. Study Objectives and Research Questions

The literature explored revealed that more research is needed on the effect of attitude, prior conceptual knowledge and instructional methods on academic achievement (Flaherty, 2020; Kahveci, 2015; Lee, 2016). Therefore, the purpose of this study was to investigate how academic achievement in chemistry could be improved using computer simulations supported by the POE strategy. The objectives of the study were to:

1. Determine the effects of computer simulations on students' attitudes towards chemistry.
2. Investigate the effects of computer simulations, attitudes and prior knowledge on the students' academic achievement.

The study aimed to answer the following research questions (RQ) to achieve these objectives:

1. What are the effects of teaching chemistry using computer simulations and conventional approaches on students' attitudes towards chemistry?
2. What are the influences of attitudes, students' prior conceptual knowledge and computer simulation instruction on their academic achievement?

5. Study Variables

For the first objective, the independent variable was the instructional approach, which was computer simulations supported by Predict-Observe-Explain (POE) instruction or conventional instruction. The dependent variable was students' attitudes towards chemistry, while the independent variable was the instructional approach. In the second objective, the instructional approach, attitudes and prior knowledge were the independent variables, while academic achievement was the dependent variable.

6. Significance of the Study

The study has the potential to contribute to chemistry education by providing empirical evidence on factors that influence academic achievement. By understanding students' attitudes, teachers can create more engaging and effective teaching methods that may enhance learning outcomes when integrating technology into instruction (Kareem et al., 2022). The evaluation of computer simulations offers insights into integrating these educational tools for a better grasp of complex chemistry concepts. Identifying the impact of prior knowledge on academic achievement enables the development of targeted support, which can assist students with the risk of not performing as expected (Darling-Hammond et al., 2020). The findings have significance for initial teacher education as they shed light on the effects of positive attitudes towards chemistry, prior knowledge and the use of simulations on students' learning outcomes.

7. Method

7.1 Research Design and Sampling

The research was a mixed-method study. The quantitative phase involved a quasi-experimental, non-equivalent control group design. Two intact grade 12 classes were randomly assigned to the experimental group (EG) and the control group (CG). These classes were sampled from two different secondary schools. The experimental group comprised 53 students, and the control group comprised 65 students. The researchers were granted ethical clearance to conduct the study by the university research ethics committee, and permission was sought and obtained from the Department of Basic Education. Informed consent was obtained from the parents or guardians of the participants.

7.2 Study Instruments for Prior Conceptual Knowledge and Attitudes

Students' prior conceptual knowledge was evaluated by administering the Chemical Kinetics Achievement Test (CKAT) to the EG and the CG as a pre-test two weeks before treatment. The CKAT test had thirty multiple-choice items (Appendix C) and was administered for one hour. Immediately after writing this test, the Attitude Towards Chemistry Scale (Appendix B) was administered to both groups for 15 minutes.

7.3 Teaching

Both groups were then taught the topic of Chemical Kinetics for one week. The experimental group was taught this topic using computer simulations and supported by the Predict-Observe-Explain strategy. The control group was taught using the conventional instructional approach.

7.4 Academic Achievement and Attitude after Treatment

Two weeks after treatment, the CKAT was administered to both classes for one hour to collect the academic achievement data. Immediately after writing the CKAT, the Attitude Towards Chemistry Lessons Scale was administered to both groups.

7.5 Attitudes towards Chemistry Lessons Scale

The Attitude Towards Chemistry Lessons Scale (ATCLS) was developed by Cheung (2009a). To examine the construct validity of the ATCLS, the researchers carried out confirmatory factor analysis (CFA, which showed that the ATCLS had four dimensions - liking for chemistry theory lessons (LCST), liking chemistry laboratory work (LLW), evaluative beliefs about school chemistry (EBSC), and behavioural tendencies to learn chemistry (BTLC) – as hypothesised. The ATCLS was used in several previous studies (Cheung, 2009b, 2011; Heng & Karpudewan, 2015) and data on its validity and reliability were reported in these studies, enhancing its suitability. A scale is reliable if it has an alpha value greater than .70 (Tavakol & Dennick, 2011). The reliability of the four dimensions in the ATCLS was examined using SPSS Statistics version 28, and Cronbach's alpha values are displayed in Table 1. The alpha values confirmed that the reliability of the ATCLS was acceptable.

Table 1: Reliability statistics

Dimension	No. of items	Alpha (α)
LCLT	3	0.77
LLW	3	0.85
EBSC	3	0.75
BTLC	3	0.79

7.6 Academic Achievement Test

The researchers developed the CKAT by choosing suitable questions from the previous grade 12 final examination questions. A panel of four qualified and experienced chemistry teachers were asked to rate the suitability of these items in the content validation of the CKAT. The feedback from this panel was used to modify items they thought needed clarity. The researchers administered the CKAT to a sample of seventy-six students who were not part of the main study, then readministered the same test two weeks later to the same sample in the pilot phase to determine the test-retest reliability (Al-Ali & Gaber, 2023). Pearson correlation was used to determine the test-retest reliability and found a statistically significant correlation in the students' marks in the first and second test administration ($r(74) = 0.81$, $p < .01$). Therefore, the results showed that the test was reliable.

7.7 Assumptions of Multiple Linear Regression Analysis

Before carrying out the multiple linear regression analysis, the researchers checked that the assumptions for multiple linear regression were not violated. These assumptions, as discussed by Williams et al. (2019), are linearity of parameters (dependent variable is assumed to be a linear function of the parameters - β_1, β_2, β_3 ...), zero conditional means of errors, homoscedasticity of errors, normal distribution of errors, predictor variables are measured without errors, absence of multicollinearity and absence of outliers.

The casewise diagnostics function in SPSS was used to identify outliers. One case was identified as an outlier and removed, reducing the sample size to 117. The sample size was appropriate as there were 20 times more cases than the independent variables (Tabachnick & Fidell, 2013). The assumption of the linearity of the relationship between the dependent variable and independent variables was tested by examining residual plots (Appendix 1). The residuals were scattered randomly around the residual = 0 line, suggesting a reasonable linear relationship. All the data points were within ±3 standard deviations along both axes, indicating a linear relationship between the dependent and the independent variables. The homogeneity of variance assumption (homoscedasticity) was confirmed by visual inspection of the scatterplots, which showed an approximate consistent spread of residuals across the range of predicted values (Appendix 1).

There was no multicollinearity of independent variables as all the variance inflation factors were less than 10, and multicollinearity tolerance values were more than 0.1. The Durbin-Watson value of 2.163 was between 1.5 and 2.5, confirming the independence of errors. The assumption of normal distribution of errors was assessed by visual inspection of the histogram of standardised residuals and normal P-P plots. This inspection confirmed the normal distribution of errors. The analyses suggested that the assumptions of multiple linear regression were not violated.

7.8 Qualitative Data Collection

Qualitative data were collected from five participants to understand the quantitative results using semi-structured interviews one week after instruction. The merits of the semi-structured interviews are that they provide an in-depth understanding of phenomena from the participants' point of view and enable data triangulation (Mwita, 2022). The researchers were granted permission by the five purposively sampled participants to record the interviews, and an audio recording device was used. Participants were informed that their identities would not be revealed so as to ensure anonymity. Each interview was performed at the student's school and lasted approximately 35 minutes. Each interview was transcribed verbatim and then checked for errors several times. Thematic analysis was used to analyse the data.

8. Findings

8.1 Effects of Teaching Using Computer Simulations and Conventional Instruction on Students' Attitudes

To answer the first research question, an independent samples *t*-test was performed. The descriptive and inferential statistics for the pre-test results obtained from the Attitude Towards Chemistry Lessons Scale are shown in Table 2.

Table 2: Statistics of the pre-test results of the students' attitude

Group	N	M	MD	SD	*t*	*P**	*df*
Experimental	53	28.58	0.53	7.98	0.38	0.71	116
Control	65	29.11		6.97			

*Statistically insignificant at $p < .05$ MD = mean difference, SD = standard deviation

The independent samples *t*-test was performed to determine if there was a statistically significant difference in the attitude of the students in the experimental group and the control group before treatment (Table 2). The results showed no statistically significant difference in students' attitudes before treatment ($t = 3.80$, $p > .05$), confirming that the students' attitudes were the same. The descriptive and inferential statistics for the post-test results from the Attitude Towards Chemistry Lessons Scale are summarised in Table 3.

Table 3: Statistics of the post-test results of the students' attitude

Group	N	M	MD	SD	*t*	*P**	*df*	Cohen's *d*
Experimental	53	36.62	6.88	5.93	-5.68	< .001	116	1.052
Control	65	29.74		7.01				

*Statistically significant at $p < .05$

The results of the independent samples t-test in Table 3 show that there was a statistically significant difference in the attitudes of students after treatment in favour of the experimental group ($t = 5.682$, $p < .05$). The results showed that teaching chemical kinetics using computer simulations improves the attitude of students towards chemistry compared to teaching the same topic using the conventional approach. The results also showed that the effect size was large ($d = 1.052$).

This finding was supported by one of the themes that emerged from the qualitative data analysis. All participants reported that they enjoyed learning chemical kinetics using computer simulations. Some of the quotes from the participants that supported this are as follows:

> *"For my case, I enjoyed it because I saw those things like those particles reacting and also, besides understanding, it was funny."* (Learner L3)
>
> *"Yes, I enjoyed that. Looking at those particles colliding and doing such things it was like that was for real. It helped me a lot in improving my chemistry."* (Learner L5)

This suggested that improving students' attitudes towards chemistry could be due to the enjoyment of learning using computer simulations.

8.2 Predictive Effects of Prior Knowledge, Computer Simulation Instruction and Attitude on Students' Academic Achievement

To answer the second research question, multiple linear regression analysis was used to examine the relationship between students' academic achievement, attitude towards chemistry, prior knowledge, and instructional strategy. The stepwise multiple linear regression procedure included prior knowledge, instructional method, and attitude in the final model. Table 4 summarises stepwise multiple linear regression analysis with the predictor variables being attitudes towards chemistry, prior knowledge and instructional strategy.

Table 4: Summary of stepwise multiple linear regression model

	B	Std. error	β	t	p
Intercept	1.668	1.333		1.251	0.214
Prior knowledge	0.724	0.108	0.486	6.712	<.001
Attitude	0.092	0.041	0.181	2.248	0.027
Instructional method	3.004	0.617	0.398	4.886	<.001
$R^2 = 0.428$ Adj $R^2 = 0.413$ $F(3.133) = 28.22$; $p < .001$					

The results showed that 41.3% of the variance in academic achievement was accounted for by prior knowledge, instructional method and attitude respectively, $F(3.133) = 28.22$, $p < .001$. Looking at the unique individual predictors, the results revealed that all three variables were statistically significant predictors of academic achievement (prior knowledge: $\beta = 0.49$, $t = 6.712$, $p < .001$, attitude: $\beta = 0.18$, $t = 2.248$, $p = 0.027$, and instructional method: $\beta = 0.40$, $t = 4.886$, $p < .001$) at the .05 level of significance. Regarding instructional methods, the results suggested that the students taught using computer simulations were more likely to have greater academic achievement than those taught using the conventional approach. Furthermore, these results indicated that students with greater conceptual knowledge and positive attitudes towards chemistry were likelier to experience greater academic success in chemistry. The effect size of the model was calculated using Cohen's f, which was found to be 0.865, which was a large effect size.

The most important predictor was prior knowledge with the largest β value, which implied that for every unit increase in prior knowledge, academic achievement increased by 0.49, closely followed by instructional approach with a β value of 0.4. The least important predictor was attitude, which only accounted for a 0.18 increase in academic achievement per unit increase in attitude.

The themes that emerged from the semi-structured interviews shed light on the findings. The first theme of conceptual understanding was that computer simulations help understand chemical phenomena at the sub-micro level of representation. Most students stated that computer simulations enabled them to observe what happens at the sub-micro level, facilitating their understanding. Some of the quotes from the students were:

> *"Computer simulations are better ... because in computer simulations I can actually visually see the particles colliding and the rates of reaction increasing in the presence of a catalyst, yeah things like that."* (Learner L1)

> *"... when you see something on the screen rather than reading in a book it's easy, when you see the particles move and everything that goes on in action, it's more understandable."* (Learner L2)

This confirmed that the use of simulations in teaching Chemical Kinetics concepts enabled students to gain conceptual understanding through visualisation, and this understanding led to an increase in academic achievement. Most students fail to understand chemistry concepts due to difficulties in linking the macro level to the sub-micro level. Using simulations enabled them to observe what occurs at the sub-micro level, and as stated by the students, this helps them understand.

The second theme was that teachers should mediate learning. Students expressed the view that computer simulations should be used together with the explanations from the teacher.

> *"When we are doing this, or they want to show us the collision theory, yeah, but when coming to other modules … like when you need to explain chemistry, we will need our teacher to explain to understand."* (Learner L4)
>
> *"... explaining using computer simulations will help me on how to know the behaviour of those particles we had been talking about to have some additional ideas to know what the teacher is talking about exactly."* (Learner L3)

The last theme that emerged on how computer simulation instruction affects students' understanding is that scaffolding prompts such as the Predict-Observe-Explain strategy help students when learning using computer simulations. Students believed that it was not just computer simulations per se that made them understand the Chemical Kinetics concepts but the Predict-Observe-Explain strategy that was used together with the simulations.

> *"Yes ... because my predictions actually were correct or almost correct, and the observations I made were recorded and marked. When explaining, I was able to grasp the correct ideas."* (Learner L1)
>
> *"The observations from the simulation helped me to see if my prediction was correct, then when I was wrong, I could understand why I was wrong, then I corrected myself."* (Learner L5)

The findings suggested that computer simulation teaching improves students' attitudes towards chemistry. The improved attitude, prior knowledge and instructional method collectively positively impact academic success.

9. Discussion

Findings from technology-aided instruction, such as computer simulations, suggest that these instructional approaches significantly affect the attitudes of students (Savelsbergh et al., 2016; Sugano & Nabua, 2020). However, the effects of studies differ in the effect sizes, which range from medium to high. A large effect size was obtained in this study, a result that is supported by Sugano and Nabua (2020). This large effect size could have been due to combining computer simulations with the POE activities.

The study also found that using computer simulations in teaching significantly predicts students' academic achievement with a β value of 0.40, which was large. This suggested that computer simulations helped students understand Chemical Kinetics concepts. This was supported by the finding that using simulations in teaching chemistry enables students to observe chemical phenomena at the sub-micro level, and this helped them gain conceptual understanding. These findings are aligned with the study by Nja et al. (2022), which revealed that flipped class teaching improves both students' academic performance and attitudes in chemistry, although this study involved university students together.

Attitude towards chemistry was found to be a significant predictor of students' academic achievement. This result aligns with previous studies (Aguilera & Perales-Palacios, 2020; Ozel et al., 2013; Vilia et al., 2017). Vilia et al. (2017) found that positive attitudes towards physics-chemistry are associated with improved academic achievement. However, while they found that attitude accounted for higher proportions of students' grade variations, our model showed that attitude had the most minor effect on academic achievement. Ozel et al. (2013) also found that, while attitude significantly predicts students' academic achievement in science, the effect size was small. The low effect sizes and low levels of variance that they explain on academic achievement do not make attitude less critical. Instead, teachers should aim to improve students' attitudes towards chemistry or other specific disciplines of science (Aguilera & Perales-Palacios, 2020). Apart from playing a role in improving students' academic achievement, attitudes also play a role in the decisions that students make when deciding on future careers or university courses.

In addition to attitudes as predictors of academic achievement, the effects of students' prior knowledge on their academic achievement were investigated in the current study. The finding that prior knowledge was the most significant predictor of academic achievement is in line with previous studies (Binder et al., 2019; Seery, 2009; Sibomana et al., 2021). For example, Seery (2009) studied the effect of undergraduate students' prior knowledge on exam performance and found a strong correlation between students' prior knowledge and exam performance. Similarly, Binder et al. (2019) studied how different types of prior knowledge predict undergraduate academic achievement in biology and physics. They found that, in biology, prior knowledge of principles and concepts could predict academic achievement, while in physics it could be predicted by prior knowledge of principles, concepts and problem-solving. Sibomana et al. (2021) suggest that teaching strategies should consider the students' prior knowledge, and hence learning should start from simple to complex. Conceptual integration and meaningful learning occur by relating new concepts to students' prior knowledge (Taber, 2015) when learning starts from the known to the unknown.

10. Limitations of the Study

The study had limitations that could have constrained the generalisability of the findings. The limitations included the fact that the study was conducted using only one grade level at the secondary school. Further studies are required to find if similar results can be obtained across different academic levels. Cultural contexts may also influence the findings; therefore, research should be pursued with students of various backgrounds. The variability among the two classes and the schools where the study was conducted is a limitation that constrains the generalisability of the findings, making it necessary to generalise the results with caution.

11. Conclusions and Recommendations

The study demonstrated that using computer simulations supported by the POE strategy in teaching chemistry improves students' attitudes towards chemistry and academic achievement compared to conventional instruction, confirming findings from previous studies. The improved attitude is associated with increased academic achievement, but the improved attitude only appears to account for a small proportion of the variance in academic achievement. When compared to the conventional approach, the use of computer simulations in instruction appears to be the factor that accounts for a more significant proportion of variance in academic achievement. However, the students' prior conceptual knowledge was the most significant predictor of academic achievement, suggesting that students with higher prior knowledge at the beginning of instruction seem to have the greatest academic achievement at the end. Previous studies also confirmed that prior knowledge is essential in improving academic achievement.

The implications of these findings are that governments should consider allocating more resources to make high-quality simulations available for teaching chemistry, especially in resource-constrained environments, to ensure equity in education. Policymakers should consider the professional development of in-service teachers in integrating computer simulations into instruction. Future studies are required to investigate the long-term effects of computer simulations on attitudes and academic achievement.

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Conflict of Interest

The authors declare that no conflict of interest exists.

Informed Consent

Informed consent was obtained from the parents/guardians of the participants involved in the study.

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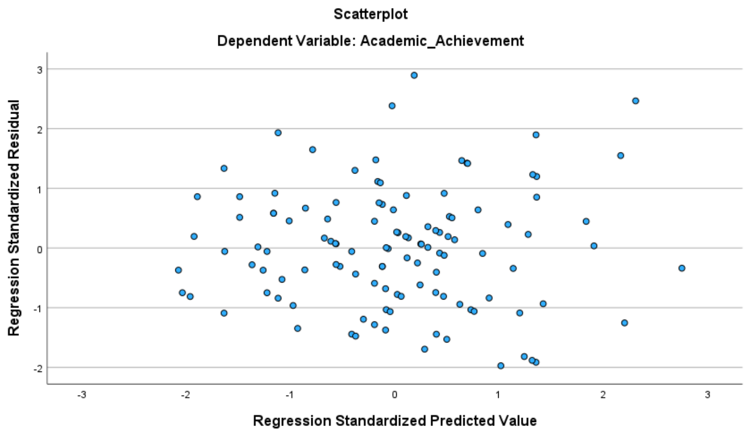
Appendix 1: Scatterplot used to test assumptions of linearity and homoscedasticity



Appendix 2: Attitudes Towards Chemistry Lessons Scale (ATCLS)

Subscale	Items	Strongly disagree	Disagree	Agree	Strongly agree
		1	2	3	4
Liking chemistry theory lessons	Q1. I like chemistry more than any other school subject.				
	Q5. Chemistry lessons are interesting.				
	Q9. Chemistry is one of my favourite subjects.				
Liking virtual chemistry laboratory work	Q2. I like to do virtual chemistry experiments.				
	Q6. When I am working in the virtual chemistry lab, I feel I am doing something important				
	Q10. Doing virtual chemistry experiments in school is fun.				
Evaluative beliefs about school chemistry	Q3. Chemistry is useful for solving everyday problems.				
	Q7. People must understand chemistry because it affects their lives				
	Q11. Chemistry is one of the most important subjects for people to study.				
Behavioural tendencies towards learning chemistry	Q4. I am willing to spend more time reading chemistry books.				
	Q8. I like trying to solve new problems in chemistry.				
	Q12. If I had a chance, I would do a project in chemistry.				

Adapted from Cheung (2011, p. 119)

Appendix 3: Chemical Kinetics Achievement Test (CKAT)

Instructions

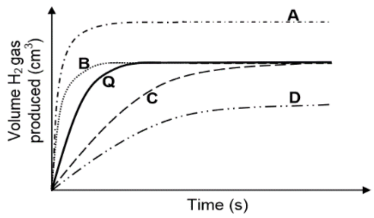
1. This question paper consists of thirty multiple-choice questions. Answer ALL questions on the separate answer sheet provided by putting a circle on the letter *A, B, C* or *D* corresponding to the correct answer.
2. For each question, indicate how confident you are of your answer by putting a circle on 1,2,3 or 4 to show whether you are *very unconfident*, *unconfident*, *confident* or *very confident*.
3. Do not write or draw anything on this question paper.
4. Do not write your name on the answer sheet.
5. Your answers will be used for research purposes only.

Time: 1 Hour

Questions

1. Graph Q (the solid line) below was obtained for the reaction of 100cm^3 of 0.1 mol.dm^{-3} HCl solution with excess magnesium powder.

Which graph (A, B, C or D) most probably represents the reaction of 100cm^3 of a 0.1 mol.dm^{-3} CH_3COOH solution with excess magnesium powder?



2. The rate of a chemical reaction can be expressed as …
   A. grams of a reactant per mole.
   B. energy consumed per mole.
   C. volume of gas formed per unit of time.
   D. moles of product per litre of solution.
3. The equation below represents the decomposition of calcium carbonate.

$CaCO_{3(s)} \rightarrow CaO_{(s)} + CO_{2(g)}$

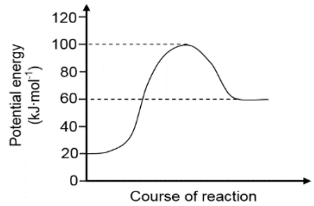
Which <u>*ONE*</u> of the following factors will increase the initial rate of decomposition of calcium carbonate?

   A. Pressure
   B. Temperature
   C. Concentration
   D. Mass of $CaCO_{3(s)}$

4. The rate of a chemical reaction is most correctly defined as …
   A. time taken for a reaction to take place.
   B. speed at which a reaction takes place.
   C. change in the amount of reactants or products.
   D. change in the amount of reactants per second.
5. Activation energy can best be described as the minimum energy required …
   A. by reactant molecules for effective collision.
   B. to make reactant molecules collide more often.
   C. to increase the kinetic energy of reactant molecules.
   D. to change the orientation of reactant molecules.
6. Which one of the following describes the effect of a positive catalyst on the net activation energy and the heat of reaction (ΔH) of a specific reaction?

	NET ACTIVATION ENERGY	ΔH
A	Increases	No effect
B	Decreases	Increases
C	No effect	Decreases
D	Decreases	No effect

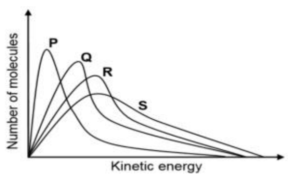
7. The temperature of a substance is a measure of the … of the particles.
   A. average potential energy
   B. average kinetic energy
   C. total kinetic energy
   D. total potential energy
8. In a chemical reaction, the difference between the potential energy of the products and the potential energy of the reactants is equal to the…
   A. enthalpy of the chemical reaction.
   B. Rate at which the reaction occurs.
   C. enthalpy change of the reaction.
   D. total potential energy of the particles.
9. The energy change during a chemical reaction is known as …
   A. bond energy.
   B. heat of reaction.
   C. activation energy.
   D. activated complex.
10. The balanced equation below represents a hypothetical reaction
    $2P(g)+3Q(g) \rightarrow 4R(g)+2S(g)$
    The rate of the reaction in terms of the number of moles of substance P used up is $1X10^{-3}$mol.dm^{3}.s^{-1}. What is the rate (in mol.dm^{-3}.s^{-1}) at which product R is formed?
    A. $1X10^{-3}$
    B. $4(1X10^{-3})$
    C. $(1X10^{-3})\div 2$
    D. $2(1X10^{-3})$
11. Consider the following potential energy diagram for a chemical reaction:



Which *ONE* of the following shows the values of the total energy change and the activation energy for this reaction?

	Energy change (kJ·mol^{-1})	Activation energy (kJ·mol^{-1})
A	80	40
B	60	100
C	40	80
D	– 40	80

12. The graphs below represent the molecular distribution for a reaction at different temperatures.

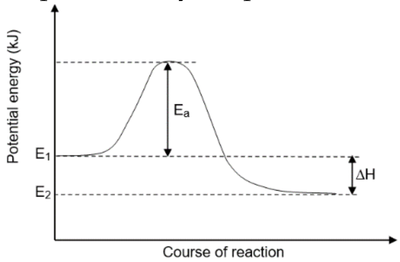


Which *ONE* of the graphs above represents the reaction at the highest temperature?

A. P
B. Q

C. R
D. S

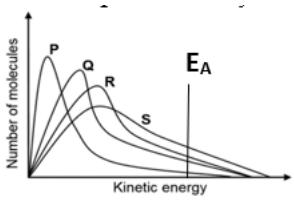
13. A certain reaction is represented by the potential energy diagram below.



Which <u>One</u> of the following quantities will change when a catalyst is added?

A. E_2
B. E_1
C. E_a
D. ΔH

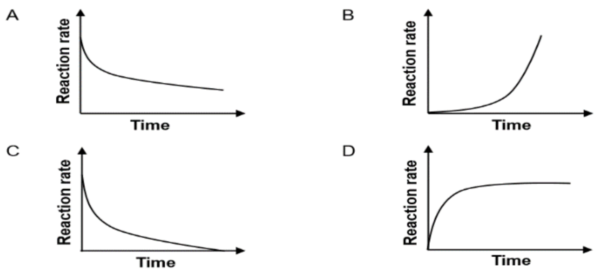
14. The Maxwell-Boltzmann energy distribution curves below show the number of particles as a function of their kinetic energy for a reaction at four different temperatures. The minimum kinetic energy needed for effective collisions to take place is represented by E_A.



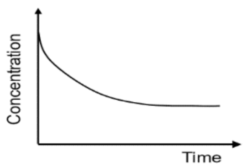
Which <u>ONE</u> of these curves represents the reaction with the lowest rate?

A. P
B. Q
C. R
D. S

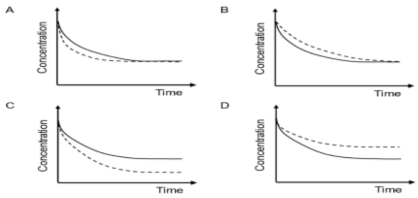
15. Which <u>ONE</u> of the reaction rate versus time graphs below best represents the reaction between magnesium and EXCESS dilute hydrochloric acid?



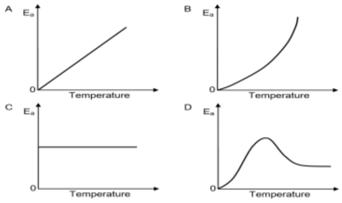
16. The graphs below represent the change in concentration of a reactant against time for a chemical reaction.



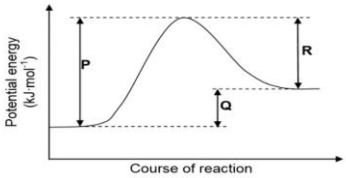
In which <u>ONE</u> of the following graphs does the dotted line show the effect of a catalyst on this reaction?



17. Which ONE of the following graphs show the relationship between the activation energy (E_a) of a reaction and temperature?



18. The energy changes represented by P, Q and R on the potential energy graph below take place during a reversible chemical reaction.



Which *ONE* of the following changes will decrease both P and R but leave Q unchanged?

A. A decrease in volume.
B. The addition of a catalyst.
C. A decrease in temperature.
D. A decrease in concentration.

19. Why does a catalyst cause a reaction to proceed faster?
    A. There are more collisions of reactants per second.
    B. The collisions of reactants occur with greater energy.
    C. The activation energy of the reaction is lowered.
    D. There are more collisions per time of greater energy.
20. Reactions are generally faster at high temperatures because the …
    A. activation energy increases.
    B. energy of the product is lowered.
    C. energy of the reactant decreases.
    D. the number of effective collisions increases.
21. Which of the following statements about reaction rate is *NOT* correct?
    A. The bigger the particle size of a solid reactant, the faster the reaction
    B. The lower the activation, the faster the reaction
    C. The higher the temperature, the faster the reaction
    D. The higher the pressure of gaseous reactants, the faster the reaction.
22. According to the collision theory, a successful collision will occur if:

I	Particles collide with the correct orientation.
II	Particles collide more frequently.
III	Colliding particles have energy greater than a certain minimum amount.

Which of the above statement(s) is/are correct?

A. I and II only
B. III only
C. I and III only
D. I, II and III

23. Consider the following reaction, which reached equilibrium in a closed vessel at a certain temperature.

$2NO_{(g)} + Cl_{2(g)} \leftrightarrow 2NOCl_{(g)}$ $\Delta H < 0$ (Exothermic)

If the temperature of the system is now *INCREASED*, it will …

A. increase only the rate of the forward reaction.
B. increase only the rate of the reverse reaction.
C. increase the rate of the forward and reverse reaction.
D. decrease only the rate of the forward reaction.

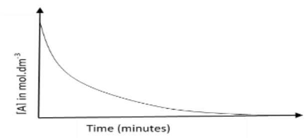
24. When the temperature of an elementary reaction increases …

A. The rate of the reaction increases if the reaction is exothermic.
B. The rate of the reaction increases if the reaction is endothermic.
C. The reaction rate increases for both exothermic and endothermic reactions.
D. The reaction rate does not change if the reaction is exothermic.

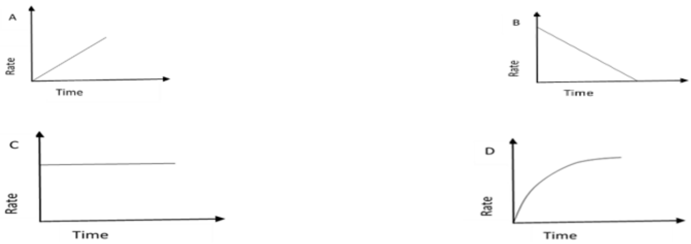
25. Two chemicals, A and B, react to form C, as shown in the equation below.

$A_{(aq)} + B_{(aq)} \rightarrow C_{(aq)}$

The graph below shows how the concentration of A changes with time



Which of the following graphs correctly shows how the rate of this reaction changes against time?



26. The gases A and B react according to the elementary reaction:

$A_{(g)} + B_{(g)} \rightarrow AB_{(g)}$

What is the effect of increasing the reaction temperature on the following?

I. Rate of collisions between reactants A and B
II. Rate of effective collisions between reactants A and B

A. Only I increase
B. Only II increases
C. Both I and II increases
D. Both I and II decreases

27. A catalyst increases the rate of a reaction by …

A. decreasing the change in enthalpy of the reaction.
B. providing an alternative reaction mechanism.
C. increasing the average kinetic energy of the reactants.
D. increasing the activation energy of the reaction.

28. The gases A and B react according to the elementary reaction:

$A(g) + B(g) \rightarrow AB(g)$.

The reaction proceeds in the presence of a catalyst. During the reaction …

A. the rate of the reaction remains constant.
B. the rate of the reaction decreases.
C. the rate of the reaction increases.

D. it is not clear how the reaction rate changes.

29. During the course of the reaction

$2N_2O_{5(g)} \rightarrow 4NO_{2(g)} + O_{2(g)}$

At time *t*, the instantaneous rate of formation of O_2 was found to be 3 mol.dm^{-3}.min^{-1}.
The instantaneous consumption rate of N_2O_5 at time *t* is equal to…

A. 1.5 mol.dm^{-3}min^{-1}
B. 3 mol.dm^{-3}.min^{-1}
C. 6 mol.dm^{-3}.min^{-1}
D. 9 mol.dm^{-3}.min^{-1}

30. During the study of the rate of the reaction:

$2A_{(g)} \rightarrow B_{(g)} + C_{(g)}$ the following data were obtained

Time (s)	0	20	40	60	80	100
[A]/mol.dm^{-3}	5.6	4.6	3.7	3.0	2.4	2.0

The average consumption rate of A, in mol.dm^{3}.s^{-1}, during the time interval between 20 s and 40 s is ….

A. -0.045
B. 0.045
C. 0.036
D. -0.036