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The Effect of Computer Simulation on Grade 11 Learners' Conceptualisation of Stoichiometric Chemistry

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ABSTRACT

This study, titled *The Effect of Computer Simulation on Grade 11 Learners' Conceptualisation of Stoichiometric Chemistry*, was carried out at a school in the Frances Baard District of the Northern Cape province of South Africa. Poor conceptualisation of stoichiometric chemistry by learners in Grades 10-12 in South Africa and, hence, their failure to apply the concepts to problem-solving in the same and other topics in chemistry, is a cause for concern. The study was conducted with the theoretical framework of activity theory. A mixed method design that consisted of a pre-test post-test experimental design, a questionnaire and interviews were used for the study. Two Grade 11 physical sciences classes which consisted of a control and experimental group were taught stoichiometric chemistry after the SCAT pre-test. The experimental group obtained an intervention comprising computer simulations during teaching, while the control group was taught using the lecture method. The ANOVA results showed that learners of the control and experimental groups were comparable in terms of prior knowledge of the topic of stoichiometric chemistry. The paired t-test showed that both groups improved their performance in stoichiometric chemistry. However, the ANCOVA results showed that the experimental group had a greater improvement in performance than the control group. The results of the SCAT post-test, observation of lessons, questionnaire and interviews showed that the experimental group conceptualised stoichiometric chemistry better than the control group. The quantitative and qualitative data was triangulated, and it also indicated that the experimental group conceptualised stoichiometric chemistry better than the control group. It is therefore suggested that using computer simulations for the teaching and learning of stoichiometric chemistry is a better method to improve its conceptualisation in the FET phase of schools in South Africa.

Keywords: stoichiometric chemistry, conceptualisation, activity theory, computer simulation, intervention

INTRODUCTION

Conceptualisation of stoichiometric chemistry is the foundation to understand the quantitative aspects of any of the topics in chemistry such as rate of reactions, chemical equilibrium, acids and bases, electrochemistry and organic chemistry (Jusniar et. al. 2019: 141; Malcolm et. al. 2018: 134; Ndlovu, 2017: 2-3). Stoichiometric chemistry deals with the study of the quantitative aspects of mass-mole relationships, chemical formulae and reactions. In chemistry, stoichiometric chemistry is a topic that is very difficult, and few learners/students like and succeed in learning it – most of them struggle to conceptualise it (Fang, Hart and Clarke, 2016: 182; Hanson, 2016:

2).Therefore, improving learners' learning and understanding of stoichiometric chemistry could possibly open doors to further studies for more students in the field of chemistry and other science-related careers (Agung and Schwartz, 2007: 4; Arya and Kumar, 2018: 2).

RATIONALE FOR THE STUDY

The National Senior Certificate examination in South Africa for Physical sciences paper 2 has questions based on application of stoichiometric chemistry concepts and the results of the examination showed that stoichiometric chemistry was performed poorly over the years. The diagnostic report recommends that learners need greater exposure in conceptualising stoichiometric chemistry for applying the concepts in the different questions where applicable (DBE, 2016, 2017; Ndlovu, 2017: 2). Malcolm *et al.* (2018: 135) argue that learners find it difficult to perform well in stoichiometric calculations, due to their lack of conceptual understanding of the mole concept, their failure to construct and balance chemical equations from a reaction given, lack of mathematical skills, and finding it difficult to interpret word problems into steps that they can proceed for problem solving in the quantitative aspects of a reaction. The ability to understand and use the mole ratio is at the heart of stoichiometry, but students lack this skill (Chandrasegaran *et al.,* 2009: 14).

Teachers need to assist learners to conceptualise stoichiometric chemistry through instruction in the classroom. However, studies conducted has reported that teachers find it difficult to teach the concepts effectively (Malcolm *et al.*, 2018: 135). The problem-solving strategies used in stoichiometry and its poor conceptualisation, have long been of concern to researchers around the world – at least since the early 1990s (Atwater and Alick, 1990: 157; Tigere, 2014: 12). Various researchers, such as Malcolm *et al.* (2018), Nkemakolam *et al.* (2018), Özmen (2008), and Rutten *et al.* (2012), all point out that using computer technology in education can help to deepen learners' understanding of scientific concepts. Develaki (2019: 10) reports that computer simulations can be incorporated into different kinds of teaching, thereby promoting students' understanding of science concepts, developing their inquiry skills and enhancing teacher education and their professional growth by recreating real-world perspectives, which, in normal classroom situations, would not be possible. In another study, by Liu (2005: 187), on making use of computer simulations, molecular animations helped students to connect chemical reactions to chemical equations when using symbols and signs. The use computer simulations to teach acids and bases, chemical bonding and chemical equilibrium also proved to have a positive effect on students' conceptualisation, achievement and also prevents misconceptions (Bayrak and Bayram, 2010: 234; Özmen, 2008: 435; Sarıçayır *et al.,* 2006: 134).

Though research has been done on the difficulties and problems learners experience learning stoichiometric chemistry and therefore performing poorly in the topic, a literature search using JSTOR, ERIC, SpringerLink, Worldwide Science, EBSCOhost and Google Scholar, on the study of teaching stoichiometric chemistry with computer simulations in Africa, did not yield any results. Therefore, considering the poor conceptualisation of stoichiometric chemistry by learners and its importance in the field of chemistry, this study seeks to determine whether using computer simulations can enhance the conceptualisation of stoichiometric chemistry.

The following null hypotheses were formulated to guide the empirical study.

$H_0$1 The learners in the control group and experimental group are not comparable in terms of their knowledge of stoichiometric chemistry.

$H_0$2 There is no significant difference between the pre-test and post-test mean scores of the Grade 11 learners in the control group.

$H_0$3 There is no significant difference between the mean pre-test and post-test scores of the of the Grade 11 learners in the experimental group.

$H_0$4 There is no significant difference between the mean post-test scores of learners in the control and experimental groups, after controlling for the effect of pre-test scores.

LITERATURE REVIEW

Stoichiometric chemistry is an important topic in chemistry that deals with the quantitative aspects of chemical change- which is the stoichiometry of a chemical reaction. (Malcolm *et al.*, 2018; Ndlovu, 2017: 2). Stoichiometric chemistry basically deals with the mole concept and its calculations with different quantities such as mass of substances, number of particles and volume. Mole is the basic unit of the amount of substance with the SI unit mol (Pekdağ and Azizoğlu, 2013: 118). Stoichiometric chemistry also involves problem solving in relation to the relationships between the number of moles of reactants and products in a chemical reaction (Hanson, 2016: 2; Okanlawon, 2010: 28). For solving problems in stoichiometry, the learner needs to do calculations on molar mass of compounds, write balanced chemical equations, apply the mole concept, determine empirical and molecular formula, use ratios in balanced equations of reactants and products, determine the limiting reagent, mass percentage and percentage yield (Gulacar, 2007: 4).

Stoichiometric chemistry is reported to be having abstract concepts and hence poorly conceptualised (Atwater and Alick, 1990: 157; BouJaoude and Barakat, 2000: 91; Bridges, 2015: 4; Fach *et al.*, 2007: 13; Schmidt, 1994: 191; Tigere, 2014: 12). As learners do not conceptualise the concepts behind stoichiometric problem-solving, they make use of algorithmic methods, and teachers even encourage them to do so. They may reach a correct answer by just memorising a formula, manipulating the formula and substituting values (Schmidt and Jignéus, 2003: 306). Researchers regard the poor conceptualisation of stoichiometric chemistry as one of the reasons that affects the interest of students in learning chemistry; researchers are also concerned that there has been a decline in the number of chemistry students at an advanced level all over the world (Broman *et al.*, 2011: 43; Fang *et al.*, 2016: 215; Malcolm *et al.*, 2018: 134).

As the traditional lecture method to teach abstract concepts does not always seem to be effective, researchers recommended using other instructional methods such as computer simulation to address the issues of learning and understanding of difficult concepts. Bailey (2007: 31) reports that students can achieve a better understanding of the relationship between the microscopic and macroscopic levels of the concepts of gases using computer animation. Udo and Etiubon (2011: 215) reports that chemistry teachers use computer simulation due to its high facilitative effect on student performance. Another study showed that the visual information provided by computer simulations helps learners to connect their understanding of chemical reactions to chemical equations (Liu, 2005: 187). Using computer-aided teaching for the topic of acids and bases had a positive effect on the achievement of students (Bayrak and Bayram, 2010: 235). Findings of the positive impact of using computer simulation to teach led Nkemakolam *et al.* (2018: 288), after conducting research on the use of computer simulation for teaching in Nigeria, to recommend that chemistry teachers should make use of computer simulation to improve students' achievement in chemistry.

Based on the reports of researchers such as Sari *et al.* (2018: 6) and Astutik and Prahani (2018: 410) that PhET simulations, when integrated in teaching and learning could enhance conceptualisation of the subject content, the same simulation was used to teach stoichiometric chemistry for the study.

THEORETICAL FRAMEWORK

For the conceptualisation of a topic such as stoichiometric chemistry, learners need to construct knowledge through activities. Hence, the study aimed to determine the effect of computer simulation on learners' conceptualisation of stoichiometric chemistry within the framework of activity theory. Activity theory helps in designing a constructivist learning environment in which learners construct their own knowledge and understanding (Singh and Yaduvanshi, 2015: 1). In the current study which consisted of an experimental group and control group, a simulation was used to teach stoichiometric chemistry to the experimental group while the control group were taught using traditional lecture method. During the lesson the experimental group learners were involved in activities based on the simulation to achieve an outcome while the control group learners involved in activities from the textbook. Hence, activity theory is appropriate as the theoretical framework for the study. Making use of visual representations can create a learning environment in which learners are able to interact with abstract concepts (Naidoo, 2017: 2). Therefore, the intentional design of the learning activities with simulations for the current study, done by interaction, can create conceptual understanding. By applying activity theory, the teacher, by using computer simulation, creates an environment that should be conducive for learners to reach their level of development.

According to the activity theory model, within the context of the study, the subject was the teachers teaching stoichiometric chemistry, the instruments were the simulations and the other teaching tools for stoichiometric chemistry, and the object or objective was the development of the various concepts in stoichiometric chemistry. In the context of the study, the tools used varied for each teacher teaching the learners. One teacher used computer simulation in addition to the whiteboard and textbook, while the second teacher used the textbook as the tool in addition to the whiteboard. The community in the activity system refers to the group of individuals who share a common objective to achieve. The communities in the study are the learners in the two classes (experimental group and control group), and their respective teachers. The subject belongs to a community that is governed by rules and divisions of roles (labour). During interaction, members of each community collaborated with each other to achieve the outcome of the activity system, which was the conceptualisation of stoichiometric chemistry (Naidoo, 2017: 4).

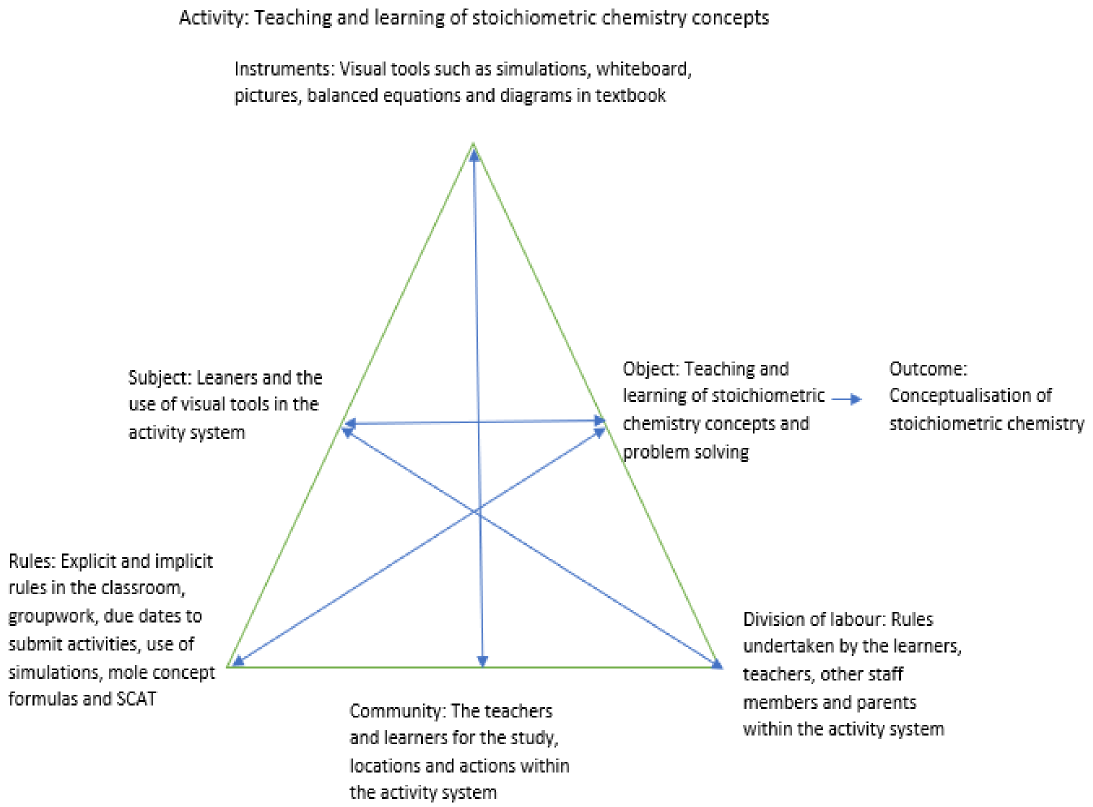


Figure 1. Adapted Activity theory model

Figure 1 emerged from this study which was adapted from the activity theory model of Engeström (Naidoo, 2017: 4). The activity system for the study is the act of teaching and learning stoichiometric chemistry with and without computer simulation. As the learners work and solve problems together within the activity system, they develop a new set of values and notions.

METHODOLOGY

Sequential experimental mixed methods design which is characterised by the collection and analysis of quantitative data in a first phase of research, followed by the collection and analysis of qualitative data in a second phase was used for the study (Subedi, 2016: 574). The explanatory sequential design is the most common and straightforward mixed methods design, whereby qualitative findings help to refine, explain and clarify the general picture presented by the quantitative results (Creswell and Creswell, 2017: 196; Maree, 2016: 316). The permission for the study was granted by the University of the Free state (Ethical clearance number UFS-HSD2018/1292) and the study formed part of the researcher's PhD project. By making use of purposive sampling learners in a school from the Frances Baard district in Kimberley, South Africa with two grade 11 classes taught by two different teachers were selected (Palinkas *et al*., 2015: 535). The two Grade 11 classes as the sample were randomly assigned as control (CG) and experimental groups (EG).

PROCEDURE FOR DATA COLLECTION AND ANALYSIS

The control group was taught stoichiometric chemistry by making use of the lecture method while the experimental group was taught the same concepts by making use of PhET computer simulations. The quantitative data for the study was collected by pre-test post-test experimental design (Creswell and Creswell, 2018: 273; Leavy, 2017: 95). A validated Stoichiometric Chemistry Achievement Test (SCAT) for the pre-test and post-test was administered on the control and experimental groups. The SCAT consisted of two main questions with sub-questions. The questions were set from the learning area of quantitative aspects of chemical change in Grade 11, adapted from past question papers for Grade 11. The questions consisted of writing balanced equations, using balanced equations to determine the limiting and excess reactants, and calculating mass and volume of products formed.

After the pre-test, lessons in stoichiometric chemistry were conducted for both control and experimental group and it was observed using an observation schedule adapted from RTOP. RTOP is an instrument that was specially designed by the Evaluation Facilitation group of the Arizona Collaborative for Excellence in the Preparation of Teachers (ACEPT) to measure reformed teaching, the idea of which is to prepare teachers to adopt a constructivist way of teaching (Kunnath, 2017: 76; MacIsaac and Falconer, 2002: 479). The observation schedule for the lesson observations of both the control and experimental groups consisted of five themes. The themes were structured to assess the degree to which the teaching took place by including aspects such as content knowledge of teacher, organisation and presentation of material, teacher- learner interaction, learner-learner interaction, opportunities for active learning with an emphasis on fundamental concepts and the incorporation of learner ideas into class trajectory. Hence the observation schedule helped to implement the study within the theoretical framework of activity theory.

For the qualitative data, self-administered questionnaire was distributed to all learners and interviews were conducted with selected learners in the study. The questionnaire required learners to complete a set of questions and to respond to related prompts after the post-test (Kabir, 2016: 208). The questionnaire consisted of 6 questions that investigated learners' understanding of stoichiometric chemistry, related calculations, and the method of teaching the lessons. Four of the six questions were based on the learners' conceptualisation of stoichiometric chemistry. The answers helped to understand whether the intervention in the experimental group had any impact on their conceptualisation. One question was based on the confidence level of the learners in stochiometric chemistry concepts. The last question was based on learners' experience of the lessons conducted in their respective groups and to determine whether the intervention with simulation helped the learners in better conceptualisation for problem solving of stoichiometric calculations.

Followed by the questionnaire, semi-structured one on one interviews with selected learners who scored the highest, middle and the lowest marks from both groups were conducted. The interview provided an elaborated in depth understanding of the learners' conceptualisation of stoichiometric chemistry and the teaching methods used for the lessons which helped to corroborate data that was gathered from the pre-test post-test and questionnaire. The interview consisted mainly of questions related to the learners' understanding of the quantitative aspects of chemical change, the importance of balancing a chemical equation for performing calculations in a chemical reaction, how well their respective lessons helped to conceptualise stoichiometric chemistry in Grade 11, and helped them to answer the post-test. The interview questions were sequenced logically and clarified during the interview where necessary. The interviews were audio recorded with the consent of the learners. This helped to explore and probe these topics and to collection in-depth, reliable and comparable qualitative data (Kabir, 2016: 212; Maree, 2016: 93).

The analysis of the quantitative section of the pre-test post-test design used statistical analysis with SPSS 24.0. Both descriptive and inferential analysis of the quantitative data obtained from the pre-test and post-test was done. The lesson observation schedule was analysed according to each criterion and the findings are provided in **Table 8**. The test response analysis was used to assess the depth of content knowledge gained by learners, and whether conceptual and or procedural knowledge was acquired and thereby, they could understand the level of conceptualisation of the content taught (Sapire, Shalem, Wilson-Thompson and Paulsen, 2016: 4–6). The answers for each question in the pre-test and post-test by learners that were selected to be interviewed were analysed. The analysis was done to identify the correctness and errors the learners made in the pre-test and how they answered the same question in the post- test, after the intervention. Therefore, analysis was done to compare performance on the pre-test and post-test and to determine whether any improvement in performance was due to an improvement in conceptualisation of stoichiometric chemistry concepts.

Thematic analysis of the open-ended questions in the questionnaire and the semi structured interview was also done. The same procedure was used for the thematic analysis of the questionnaire and the interview and is given below.

- Step 1: Familiarising with the responses written by the participants by reading through it several times and reflecting on its overall meaning. The recordings of the interview were transcribed and the same step was followed.
- Step 2: Taking the text data from the responses in the questionnaire and interview, segmenting the sentences into categories and labelling the categories with a term. This step is called coding.
- Step 3: Generating a description and themes from codes. In this step, codes from the previous step were used to generate themes. These themes appeared as major findings in qualitative analysis. An inductive approach to data coding and analysis was predominantly used (Braun and Clarke, 2012:57). It is a bottom-up approach, where the content of the data collected derives the codes, which closely match the content.
- Step 4: Representing the description and themes by making use of visuals, figures or tables as adjuncts to the discussion. This step involved the final analysis step of writing and reporting.

The research instruments described above and their aim are summarised in the **Table 1**.

Table 1. Summary of research instruments

Phase	Instrument	Aim
1. Quantitative data collection	Pre-test and post-test	Numerical data
2. Qualitative data collection	Observation schedule, questionnaire, structured interview	Textual data
3. Quantitative data analysis	Descriptive and inferential analysis of pre-test post-test	Meaningful measures of quantitative data
4. Qualitative data analysis	Lesson observation analysis of both groups, pre-test post-test response analysis, thematic analysis of questionnaire and interviews of the same learners	Qualitative explanation of results

Table 2. ANOVA results of the pre-test

	ANOVA- Pre-test						
	Mean scores	**SD**	**Sum of squares**	**df**	**Mean square**	**F**	**Sig.**
Control group	23.87	21.179					
Experimental group	19.63	15.521					
Between groups			5498.667	10	549.867	1.391	.257
Within groups			7508.800	19	395.200		
Total			13007.467	29			

Table 3. Means and SD for pre-test and post-test of control group

SCAT	Mean	N	SD
Pre-test	23.87	30	21.179
Post-test	41.20	30	28.924

Table 4. Paired samples t-test for control group

	Paired difference						
	Mean	**SD**	**95% confidence interval of the difference**		**t**	**df**	**Sig. (2-tailed)**
			Lower	**Upper**			
Pre-test-Post-test	-17.33	21.485	-25.536	-9.311	-4.419	29	.000

RESULTS OF THE PRE-TEST AND POST-TEST OF CONTROL AND EXPERIMENTAL GROUP

The means, modes, medians and standard deviation for the pre-test were calculated. ANOVA was used to determine whether the learners in the two groups were comparable in terms of their knowledge of the topic of stoichiometric chemistry. It was found that there was no significant difference in the pre-test scores at $p < 0.05$ level for the two groups [$F (10, 19) = 1.391$, $p = .257 > 0.05$]. The null hypothesis ($H_0 1$) which stated that the learners in the control group and experimental group are not comparable in terms of their knowledge of stoichiometric chemistry is, thus, rejected. The probability is that the two groups were comparable in terms of their knowledge of the topic of stoichiometric chemistry. **Table 2** represents the ANOVA results of the pre-test.

Paired t-Test

The paired sample t-test was conducted to find out if there was a significant difference between the mean scores of the pre-test and post-test of the control group and experimental group. Means and standard deviation (SD) for the pre-test and post-test of the control group were calculated (see **Table 3**). It was observed that the control group had improved from the pre-test to (Mean = 23.87, Standard Deviation = 21.179) to the post-test (Mean = 41.20, Standard Deviation = 28.924).

From **Table 4**, it can be observed that there is a significant difference between the pre-test and post-test scores of the control group ($t (29) = -4.419$, $p < 0.05$, Sig. (2-tailed) = .000). As the p value is < 0.05, the probability is, thus, greater that there is some significant difference between the pre-test and post-test mean scores of the control group. The null hypothesis ($H_0 2$) is, thus, rejected.

Means and standard deviation (SD) for the pre-test and post-test of the experimental group were calculated (see **Table 5**). It was observed that the experimental group had improved from the pre-test (Mean = 19.63, Standard Deviation = 15.521) to the post-test (Mean = 52.94, Standard Deviation = 20.66).

Table 5. Means and SD for pre-test and post-test for experimental group

SCAT	Mean	N	SD
Pre-test	19.63	32	15.521
Post-test	52.94	32	20.666

Table 6. Paired samples t-test for experimental group

	Paired difference						
	Mean	SD	95% confidence interval of the difference		t	df	Sig. (2-tailed)
			Lower	Upper			
Pre-test-Post-test	-33.313	19.633	-40.391	-26.234	-9.598	31	.000

Table 7. ANCOVA summary of achievement by control group and experimental group

Tests of between subject effects						
Dependent variable: Post-test						
Source	**Type III sum of squares**	**Df**	**Mean square**	**F**	**Sig.**	**Partial Eta squared**
Corrected model	15141.473	2	7570.736	18.237	.000	.382
Intercept	22332.658	1	22532.658	54.279	.000	.479
Pre-test	13008.277	1	13008.277	31.336	.000	.347
Group	3491.589	1	3491.589	8.411	.005	.125
Error	24492.398	59	415.125			
Total	178100.000	62				
Corrected Total	39633.871	61				

a. R Squared =.382 (Adjusted R squared = .361)

The results in Table 6 showed that there is a significant difference between the pre-test and post-test scores of the experimental group ($t\ (31) = -9.598$, $p < 0.05$, Sig. (2-tailed) = .000 (p value < 0.05)), and, hence, the null hypothesis H_03, which stated that there is no significant difference between the mean pre-test and post-test scores of the experimental group, is rejected.

ANCOVA

ANCOVA (Analysis of Covariance) was used to find out whether there is any significant difference between the group means of the SCAT administered for the two groups. The lecture teaching method for the control group and the use of computer simulations for the intervention with the experimental group were the independent variables for the one-way ANCOVA. The post-test scores were the dependent variables and the pre-test scores were used as the covariate to control for individual difference.

The result of the ANCOVA is that there is a significant effect of the covariate, which is the pre-test, as $F\ (1,61) = 31.336$, $p < 0.05$, Sig. value = .000. Moreover, the result shows that the instructional method had a significant effect (Group), as $F\ (1,61) = 8.411$, $p < 0.05$, Sig. value = .005 (p value < 0.0). The ANCOVA results show that there is a statistically significant difference between the mean post-test scores of learners in the control and experimental groups. Therefore, the null hypothesis (H_04), which states that there is no significant difference between the mean post-test scores of learners in the control and experimental groups, after controlling for the effect of pre-test scores, is rejected.

PRACTICAL SIGNIFICANCE AND EFFECT SIZE

The effect size using Cohen's *d* was calculated to assist in drawing conclusions on the practical significance. For the study, Cohen's *d* was determined by calculating the mean difference between the post-test scores of the two groups, and then dividing the result by the pooled SD, using the formula given below.

$$\text{Cohen's } d = (M_2 - M_1) / SD_{pooled}$$

where

$$SD_{pooled} = \sqrt{((SD_1^2 + SD_2^2)/2)}.$$

If the Cohen's $d = 0.2$, it represents a small effect, $d = 0.5$, represents medium effect and $d = 0.8$ represents a large effect.

The Cohen's *d* was calculated as 0,46 and hence, it can be understood that the intervention for the experimental group had a medium effect and the statistical difference found between the mean post-test scores of learners in the experimental group and control group was meaningful.

DESCRIPTIVE STATISTICS

Graphical comparison of the means of the pre-test post-test results were conducted and is given below. CG represents control group and EG represents experimental group.

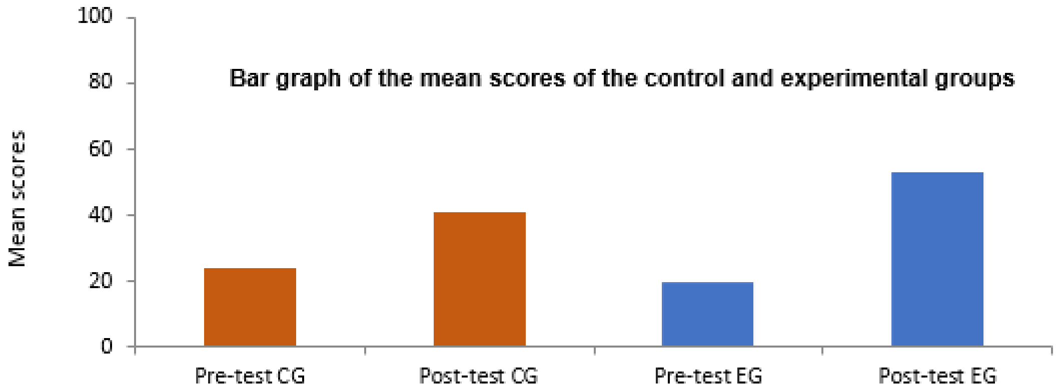


Figure 2. Bar graphs of means of the pre-test and post-test scores of the control group and experimental group

The graphical representation shows that the post-test scores for both CG and EG were greater than their respective pre-test scores. However, the mean post test score of the EG was greater than that of the CG.

RESULTS OF THE LESSON OBSERVATION

A summary of the analysis of the lesson observation conducted with the observation schedule of both control and experimental group under the different themes is presented in Table 8.

Table 8. Findings from lesson observation

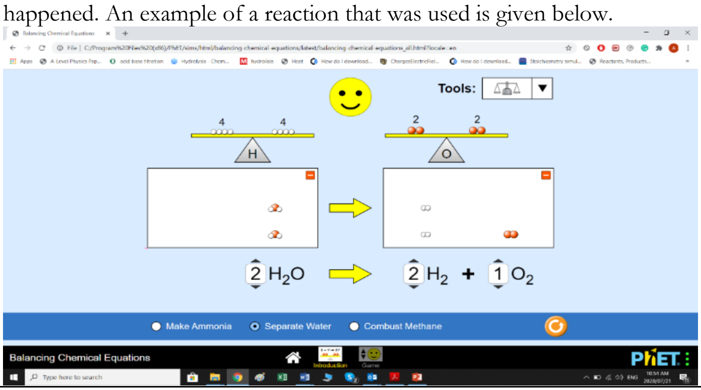
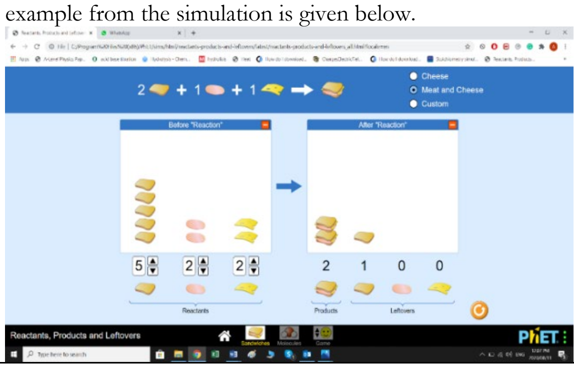
Themes	Control group	Experimental group
1. Lesson design and implementation-	For the control group, the teacher used the traditional lecture method for teaching the concepts in stoichiometric chemistry. Checking on prior knowledge was not done for all lessons. The lessons provided minimum opportunity for learners to gain active exploration experience and to interact with the teacher for problem-solving. During the lessons, the teacher wrote chemical equations on the board and asked the learners to balance the equations by manipulating the coefficients of the formula of each substance in the reaction. Steps were provided for learners to follow to perform mole ratio calculations.	For the experimental group, in all lessons the learners had the opportunity to apply their prior knowledge. Teacher–learner and learner–learner interactions were evident, and the learners could actively explore the concepts by using PhET simulations and engage in discussions, The lessons demonstrated the model for activity theory. This could have helped the experimental group to develop meaning of the content. With the PhET simulations, the learners could view the microscopic representation of each molecule in the reaction, and they could answer to the questions of the teacher. Hence it could be interpreted that representations helped them to recall their understanding of atoms and molecules and visualise each molecule and any change that happened. An example of a reaction that was used is given below. 

Table 8. Findings from lesson observation (continued)

Themes	Control group	Experimental group
2. Content knowledge of teacher, organisation and presentation of material-	For the lessons the teacher used the whiteboard and textbook as media. The lessons were observed to be mostly presented by delivering factual information. For example, the concept of using ratios to calculate the limiting reagent, amount of product formed, and leftovers, was presented by explaining how to do the calculation following certain steps.	In the experimental group, the PhET simulations, whiteboard and textbook were used as media while teaching. Except for one lesson the teacher linked the concept with real-life experiences, to achieve better conceptualisation. Real life example of making sandwich was used to teach the application of mole ratio in stoichiometric chemistry calculations. A screen shot of a real life example from the simulation is given below. 
3. Learner participation in the lesson-	The teacher used the whiteboard to explain the concepts in all lessons, and asked learners to read important points in the textbook. The learners were recalling/summarising facts and using algorithmic methods for doing the activities.	Except for one lesson, the teacher used the PhET simulations to conduct lessons based on calculations of limiting reactant, products and leftovers. It was observed that learners could view the reactants and products at the microscopic level and the leftovers of the reaction. Therefore, it could be interpreted that the molecular representation from the simulations allowed the learners to engage in critical evaluation of the content.
4. Classroom culture: learner–learner interaction-involvement of learners in communicating ideas in a variety of ways.	A few of the learners discussed in pairs and helped each other to balance equations and work on other problem-solving activities. The teacher mainly issued instructions to the learners and emphasized using the steps given to do the activities.	From the observation it was understood that the simulation gave the learners the opportunity to manipulate the game-based activities to determine the products and leftovers, and then to discuss their answers. In this way, the lessons with simulations opened doors for inquiry-based learning for problem-solving, which is likely to improve learners' ability to construct their own knowledge.
5. Classroom culture: teacher–learner interaction-	The teacher explained the various concepts to the learners, and followed up the explanation by assigning activities they had to complete. This was followed by corrections on the board by explaining the concept and the steps to follow for the complex stoichiometric calculations	In the experimental group the learners it was observed that learners had regular interaction with the teacher while they completed the activity through games to determine the products and leftovers. It was also observed that the teacher waited for the learners to provide answers for the games and, during explanations, learners were given the opportunity to engage in meaningful conversation to clear up confusion that they experienced and which caused them to make mistakes in calculations. Even though the lessons were controlled by the teacher, the learners had the freedom to interact with the teacher and to determine how the teacher could help with learning.

RESULTS OF THE TEST RESPONSE ANALYSIS OF PRE-TEST & POST-TEST

From the analysis of the responses to questions in the pre-test by the 12 interviewee learners of control and experimental groups, it was found that learners equally had challenges to balance equations. The other challenges included writing correct formulae of reactants and products, use of multiples of the actual coefficients in balanced equations, balancing by making the total number of molecules the same on both sides of the equation. Limiting reagent is a new concept in Grade 11 and, hence, neither group knew the definition for limiting reagent and its calculation. Learners in both groups could apply the mole-concept formula, which they had learned in Grade10, but could not use it for further calculations to find the number of moles when mass was given, and vice versa. Learners could not correctly apply the ratios in balanced equations to perform calculations.

The test response analysis of the post-test showed that more learners in the experimental group than the control group improved their performance and it could be interpreted that the improvement was due to learners understanding of the different concepts after the lesson. After the lessons both groups had improved in balancing equations. As mentioned above the limiting reagent and its calculations were a new topic in Grade 11, however, after the lessons there was an improvement in their understanding regarding the concept. The microscopic representations of the different reactions and the activities in the form of games in the simulations that were used for teaching and learning in the experimental group could have helped the learners to rearrange their initial understanding about the concepts in stoichiometric chemistry, thereby improving their conceptual understanding It was also observed that the learners in the control group used algorithms to do calculations, for instance, selecting a formula and substituting the data that was available.

RESULTS OF THE QUALITATIVE SECTION OF QUESTIONNAIRE AND INTERVIEWS

The interview assisted in an in depth and detailed understanding of how well the learners improved in conceptualisation of the concepts and how the teaching methods assisted in the conceptualisation. From the data analysis of the questionnaire and interview, it could be interpreted that some learners in both control and experimental groups, even after the lessons, faced challenges in applying their understanding of stoichiometric chemistry. Most responses in both questionnaire and interview by the control group showed that deep learning did not take place and they only gained factual knowledge to solve stoichiometric calculations However, the data analysis of the responses from the questionnaire and interviews showed that the lessons of the experimental group resulted in an improvement in the learners' conceptualisation of stoichiometric chemistry.

In response to questions about the teaching method, more learners in the experimental group responded that using simulations helped them to visualise the balancing of equations and to do calculations based on amount of reactants, products, limiting reagents and leftovers. Therefore, it can be interpreted that the activities in the simulations, which involved visual representations in the form of games, helped learners to construct their own knowledge. It was evident in responses to the questionnaire and in the interviews that learners in the experimental group had an improvement in conceptual and procedural knowledge about the importance of balancing equations, limiting reagents and its calculations. This conceptualisation helped the experimental group learners to explain how the calculation to determine the limiting reagent could be performed, and how they could apply it in calculations – they were better than the control group learners at explaining this. It was evident from the responses of the control group that these learners still had this misconception. The responses from the learners in experimental group showed that they gained problem solving skills in stoichiometric chemistry calculations better than the control group learners.

DISCUSSION OF RESULTS

After analysing the data, the findings from the quantitative and qualitative methods were compared and contrasted by triangulation. The two forms of data were combined by integration, which is called connecting the quantitative results to qualitative data (Creswell and Creswell, 2018: 222). This is the point of integration in an explanatory sequential design. For the study, the quantitative results from the pre-test and post-test were triangulated with the qualitative test response analysis, interviews and the questionnaire. This helped to integrate the findings of the qualitative data and the quantitative results and enhanced the trustworthiness of the research findings (Creswell and Creswell, 2018: 223). For this study, the test response analysis, interviews and the questionnaire helped to clarify, interpret and explain the results, performance and conceptualisation of the learners, as gleaned from the post-test. The quantitative data explained whether the performance of learners changed (improved) after the intervention. Thus, the qualitative data provided greater depth and insight into the quantitative results. It explained how the data from the qualitative method informed the quantitative data.

While the quantitative analysis focused on the performance of learners in stoichiometric chemistry, the qualitative analysis focused on the conceptualisation of stoichiometric chemistry. The results that emerged from the quantitative analysis of the pre-test post-test design guided the whole research process and were complemented by the qualitative analysis of the test response analysis, questionnaire and interview. **Figure 3** shows the essence of the way triangulation that was facilitated for the study.

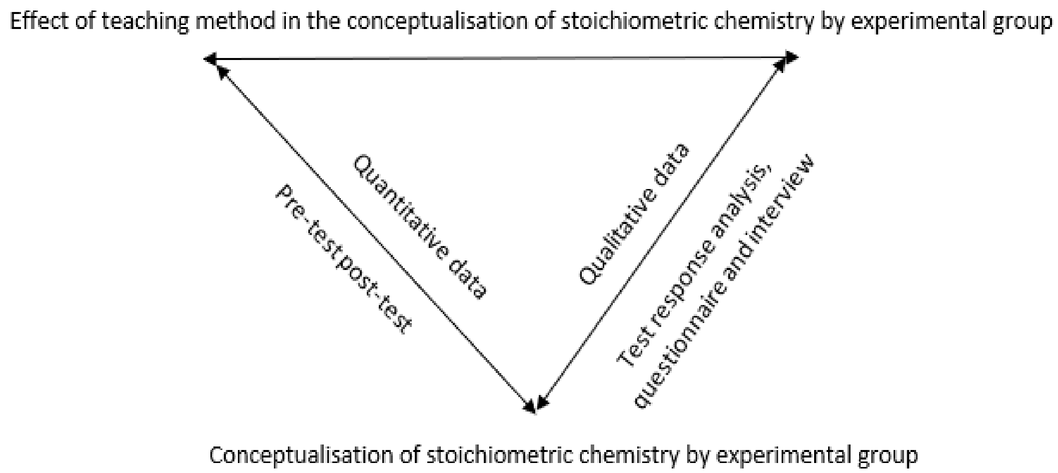


Figure 3. Triangulation of quantitative and qualitative results

The quantitative data analysis of the pre-test and post-test inductively found that both control and experimental groups improved in their performance of stoichiometric chemistry. Further analysis found that the performance improvement of the experimental group was greater than the control group. The qualitative test response analysis of the answers of the post-test supported this finding.

An inductive approach was also used for the analysis of the questionnaire and interview responses. The analysis of the qualitative questionnaire section and the interviews found that some of the learners in the control group were not satisfied with the lecture method to explain the concepts. However, most of the learners in the control group appeared satisfied with the algorithmic methods taught by the teacher for performing calculations. The teacher's use of algorithmic methods for problem solving was also noticeable during the lesson observation. It could then be interpreted that in the post-test, these learners followed the algorithmic steps to perform calculations and could not complete the calculations successfully. This interpretation is in line with researchers who has reported that the use of algorithmic methods without conceptualisation can be unsuccessful for problem solving. The interpretation concurs with their views that if conceptualisation does not occur, using algorithmic steps may fail to help a learner perform complex calculations correctly, because it comes down to applying steps without reflection and understanding.

From the findings of the interviews and questionnaire for the experimental group, it is clear that learners could interact with each other during discussions while being taught with the simulation. Moreover, the visual microscopic representations in the simulations helped many of the learners to understand the chemical reactions better. The visual representations helped them also to remember and understand what had been taught and helped them to perform better in the post-test. The rational for the study and literature review had also pointed out the positive impact of using molecular animations and visual representation with simulations for the better understanding of the different topics in chemistry. A major finding of the quantitative analysis is that the performance of experimental group learners in the post-test was better than that of learners in the control group. The interview and questionnaire analysis supports the above finding as the learners in the experimental group were better at explaining the importance of balancing equations, determining the limiting reagent, and explaining how ratios could be used to determine the limiting reagent and the amount of products formed. This finding further explains that experimental group learners had a better conceptualisation than the control group learners which resulted in a better performance in the post-test. Thus, the qualitative data that had been collected and analysed integrated with the quantitative data that had been collected and analysed, helped to develop a deeper understanding of the data and to gain a more complete picture of the study.

CONCLUSION

For further studies in chemistry, conceptualising stoichiometric chemistry plays an important role. The aim of this study, namely, to determine the effect of computer simulations on the conceptualisation of stoichiometric chemistry within theoretical framework of activity theory, was achieved. According to the activity theory model the use of visual tools which was mainly the PhET simulations, engaged the learners in activities based on chemical reactions. The interaction with simulated activities also helped the learners to construct their own knowledge thereby improving their conceptualisation of stoichiometric chemistry. From the analysis of the experimental design, questionnaire and interviews it can be concluded that there was greater improvement in learners' conceptualisation of stoichiometric chemistry in the experimental group than was the case for learners in the control group. Therefore, the study recommends the use of computer simulations for the teaching and learning of stoichiometric chemistry, as it is likely to improve its conceptualisation in the FET phase of schools in South Africa. The study further recommends a change in the teaching methods used by teachers and to integrate computer simulation to teach various concepts. Teachers may use a blended approach by making use of simulation in combination with other teaching methods, such as direct instruction, problem-solving and inductive or deductive reasoning.

The study has implications for physical sciences learners and teachers, physical sciences subject advisors, the Department of Basic Education, undergraduate chemistry students and chemistry lecturers at tertiary institutions. The study contributes to the improvement of learners' conceptualisation of stoichiometric chemistry and improved learner participation in the learning process, which makes learning science fun. Doing so might reduce the number of learners who discontinue learning physical sciences in Grades 10, 11 and 12 in South Africa due to their poor understanding and conceptualisation of stoichiometric chemistry and, hence, chemistry. Therefore, the study might contribute to producing more chemistry professionals for the chemical industry, to promote the economic growth and development of the country.

A limitation of the study was that instruments for the quantitative data collection used were not constructed to provide evidence of whether conceptualisation of the concepts took place. A well-designed quantitative questionnaire may have provided more evidence of the conceptualisation of stoichiometric chemistry. The topic of stoichiometric chemistry was dealt with at the school close to the June examinations. Hence, the teacher had to conclude the lessons and expose learners to minimum practise in solving problems using computer simulations at different difficulty levels. This could have affected the slow learners in relation to conceptualisation of the topic. Other than the guidance given by the researcher, the teacher involved in the teaching of stoichiometric chemistry using computer simulation as a tool was not given formal training by professionals on using computer simulation to teach. Formal training could have had an effect on the teacher, who may have explored simulation deeply, and used innovative ways to expose learners to the different difficulty levels of the games, while conducting the lessons. The study can be extended to a larger sample size, involving more learners doing physical sciences in the province or country, with a quantitative questionnaire to collect data. This could assist to generalise findings.

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