

University of Kentucky UKnowledge

Theses and Dissertations--Education Science

**College of Education** 

2016

## EVALUATING ROLE OF INTERACTIVE VISUALIZATION TOOL IN IMPROVING STUDENTS' CONCEPTUAL UNDERSTANDING OF CHEMICAL EQUILIBRIUM

Bharath Sampath Kumar *University of Kentucky*, bskumar80@gmail.com Author ORCID Identifier: http://orcid.org/0000-0002-3594-7881 Digital Object Identifier: https://doi.org/10.13023/ETD.2016.403

Right click to open a feedback form in a new tab to let us know how this document benefits you.

## **Recommended Citation**

Sampath Kumar, Bharath, "EVALUATING ROLE OF INTERACTIVE VISUALIZATION TOOL IN IMPROVING STUDENTS' CONCEPTUAL UNDERSTANDING OF CHEMICAL EQUILIBRIUM" (2016). *Theses and Dissertations--Education Science*. 18. https://uknowledge.uky.edu/edsc\_etds/18

This Doctoral Dissertation is brought to you for free and open access by the College of Education at UKnowledge. It has been accepted for inclusion in Theses and Dissertations--Education Science by an authorized administrator of UKnowledge. For more information, please contact UKnowledge@lsv.uky.edu.

## STUDENT AGREEMENT:

I represent that my thesis or dissertation and abstract are my original work. Proper attribution has been given to all outside sources. I understand that I am solely responsible for obtaining any needed copyright permissions. I have obtained needed written permission statement(s) from the owner(s) of each third-party copyrighted matter to be included in my work, allowing electronic distribution (if such use is not permitted by the fair use doctrine) which will be submitted to UKnowledge as Additional File.

I hereby grant to The University of Kentucky and its agents the irrevocable, non-exclusive, and royalty-free license to archive and make accessible my work in whole or in part in all forms of media, now or hereafter known. I agree that the document mentioned above may be made available immediately for worldwide access unless an embargo applies.

I retain all other ownership rights to the copyright of my work. I also retain the right to use in future works (such as articles or books) all or part of my work. I understand that I am free to register the copyright to my work.

## **REVIEW, APPROVAL AND ACCEPTANCE**

The document mentioned above has been reviewed and accepted by the student's advisor, on behalf of the advisory committee, and by the Director of Graduate Studies (DGS), on behalf of the program; we verify that this is the final, approved version of the student's thesis including all changes required by the advisory committee. The undersigned agree to abide by the statements above.

Bharath Sampath Kumar, Student Dr. Rebecca Krall, Major Professor Dr. Robert Shapiro, Director of Graduate Studies

# EVALUATING ROLE OF INTERACTIVE VISUALIZATION TOOL IN IMPROVING STUDENTS' CONCEPTUAL UNDERSTANDING OF CHEMICAL EQUILIBRIUM

## DISSERTATION

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the College of Education at the University of Kentucky

> By Bharath Sampath Kumar

Lexington, Kentucky

Director: Dr. Rebecca Krall, Associate Professor of STEM Education

2016

Copyright © Bharath Sampath Kumar 2016

## ABSTRACT OF DISSERTATION

## EVALUATING ROLE OF INTERACTIVE VISUALIZATION TOOL IN IMPROVING STUDENTS' CONCEPTUAL UNDERSTANDING OF CHEMICAL EQUILIBRIUM

The purpose of this study is to examine the role of partnering visualization tool such as simulation towards development of student's concrete conceptual understanding of chemical equilibrium. Students find chemistry concepts abstract, especially at the microscopic level. Chemical equilibrium is one such topic. While research studies have explored effectiveness of low tech instructional strategies such as analogies, jigsaw, cooperative learning, and using modeling blocks, fewer studies have explored the use of visualization tool such as simulations in the context of dynamic chemical equilibrium. Research studies have identified key reasons behind misconceptions such as lack of systematic understanding of foundational chemistry concepts, failure to recognize the system is dynamic, solving numerical problems on chemical equilibrium in an algorithmic fashion, erroneous application Le Chatelier's principle (LCP) etc. Kress et al (2001) suggested that external representation in the form of visualization is more than a tool for learning, because it enables learners to make meanings or express their ideas which cannot be readily done so through a verbal representation alone. Mixed method study design was used towards data collection. The qualitative portion of the study is aimed towards understanding the change in student's mental model before and after the intervention. A quantitative instrument was developed based on common areas of misconceptions identified by research studies. A pilot study was conducted prior to the actual study to obtain feedback from students on the quantitative instrument and the simulation. Participants for the pilot study were sampled from a single general chemistry class. Following the pilot study, the research study was conducted with a total of 27 students (N=15 in experimental group and N=12 in control group). Prior to participating in the study, students have completed their midterm test on the topic of chemical equilibrium. Qualitative interviews pre and post revealed students' mental model or thought process towards chemical equilibrium. Simulations used in the study were developed using the SCRATCH software platform. In order to test the effect of visualization tool on students' conceptual understanding of chemical equilibrium, an ANCOVA analysis was conducted.

Results from a one-factor ANCOVA showed posttest scores were significantly higher for the experimental group ( $M_{\text{postadj.}} = 7.27 \ SD_{\text{post}} = 1.387$ ) relative to the control group ( $M_{\text{postadj.}} = 2.67, SD_{\text{post}} = 1.371$ ) after adjusting for pretest scores, F(1,24) =71.82,  $MSE = 1.497, p = 0.03, \eta_p^2 = 0.75, d = 3.33$ .

Cohen's d was converted to an attenuated effect size d\* using the procedure outlined in Thompson (2006). The adjusted (for pretest scores) group mean difference estimate without measure error correction for the posttest scores and the pretest scores was 4.2 with a Cohen's d = 3.04.

An alternate approach reported in Cho and Preacher (2015) was used to determine effect size. The adjusted (for pretest scores) group mean difference estimate with measurement error correction only for the posttest scores (but not with measurement error correction for the pretest scores) was 4.99 with a Cohen's d = 3.61. Finally, the adjusted (for pretest scores) group mean difference estimate with measurement error correction for both pretest and posttest scores was 4.23 with a Cohen's d = 3.07. From a quantitative perspective, these effect size indicate a strong relationship between the experimental intervention provided and students' conceptual understanding of chemical equilibrium concepts. That is, those students who received the experimental intervention had exceptionally higher

KEYWORDS: Chemical Equilibrium, Visualization, Alternate Conceptions, Ontological Shift. Simulations

Bharath Sampath Kumar

## <u>10/20/2016</u>

# EVALUATING ROLE OF INTERACTIVE VISUALIZATION TOOL IN IMPROVING STUDENTS' CONCEPTUAL UNDERSTANDING OF CHEMICAL EQUILIBRIUM

By

Bharath Sampath Kumar

Dr. Rebecca Krall Director of Dissertation

Dr. Robert Shapiro Director of Graduate Studies

October 20, 2016

## (DEDICATION)

Dedicated to the memory of my Father Late Shri, P. Sampath Kumar 1953-2002

And

Beloved mother, friend and mentor, Mrs. Malathy Sampath Kumar

#### ACKNOWLEDGEMENTS

I would like to express my sincere gratitude and thanks to Dr. Rebecca Krall (Associate Professor, STEM Education), who is my research advisor and committee chair. Dr. Krall many thanks to you for your support and guidance. I remember writing an assignment during the first semester in your class. I did not know back then, the assignment would turn in to a dissertation, but you were always in the background pushing me to pursue the area of chemical equilibrium misconceptions. I do not have sufficient words to thank you enough for your contribution.

I would like to take this opportunity to thank the rest of the committee members, Dr. Michael Toland, Dr. Brett Criswell and Dr. Stephen Testa. Your time, effort and continuous support and feedback meant a lot. Without all your support, the dissertation wouldn't have been possible. Many thanks to you all for being the awesome committee members. I could not have asked for a better group of committee members.

I would also like to extend my sincere thanks to Dr. Patric Spence for his willingness to serve as the outside examiner.

I would also like to give special thanks to general chemistry course instructors Dr. Lisa Blue, Dr. Kim Woodrum and Dr. Chad Risko. Many thanks to you all for letting me in to your classroom and offering me precious time during your class, so I can talk to students about my research. I also wanted to thank you all for taking your time to provide feedback on the quantitative instrument used in the study.

I would like to extend my sincere gratitude to all participants. Thank you all. Without your support and feedback, this study would have just remained a dream. Your support provided life to the research. I could witness your spirit through the qualitative interviews. Once again, many thanks to all participants.

I would like to thank Dr. Sumit Das (Chair, Department of Physics) and Dr. Michael Cavagnero (Former Chair, Department of Physics) and Mr. Steve Ellis (Instructor, Department of Physics) for their financial support through teaching assistantship during the first two years of my graduate program. I would also like to extend my sincere thanks to all the office staff in the Department of Physics, in particular Carol Cottrell.

I would like to thank Dr. Laurie Henry (Associate Dean, College of Education), Dr. Jennifer Wilhelm (Chair, STEM Education), Dr. Rebecca Krall and Dr. Jessica Hearn (Director, UKY Evaluation Center) for their financial support during the last two years of my graduate program. I would like to thank the office staff in STEM Education and Curriculum and Instruction. In particular, I would like to thank Betty McCann and Tonya Sleet Brooks.

I would also like to extend special thanks to Roda Ferraro. Thank you Roda for spending your valuable time offering feedback on the qualitative piece.

I would also like to thank Dr. Neomia Hagans (Regional Coordinator, Robinson Scholar Program, UKY) for her generous support during the summer session. The experience I received through the Robinson Scholar program was remarkable. I am glad, I would be able to work as an instructor for them this summer (2016). I wish the program and students who would continue to benefit through the program in the future, all the very best.

iv

I would also like to thank Mrs. Julie Lane Bond for rendering her alluring and lovely voice that added a whole new dimension to my simulations. Julie, many thanks. Students consistently suggested in their feedback, the voice was clear and audible. Many thanks to Steven Bond, Alec Bond, Buddy, Huckleberry and Blueberry.

I would also like to thank the University of Kentucky and the Graduate school for providing me with a high quality education.

It's time to thank family members. They have stood beside me during hard times including financial hardships and have continued to support me to pursue my dreams. I would like to thank my brother-in-law Mr. Sudarsanan Ranganathan, my loving and caring sister Mrs. Sunitha Sudarsanan and their awesome kids Saarang and Sashank.

Last but not least, I would like to thank my mom Mrs. Malathy Sampath Kumar. There's no one who has stood beside me all these years like her. I have never seen a woman more strong willed and confident than her. In my view she's the strongest, honest person and most beautiful at heart, I have come across in my 36 years of life. Without her blessings and best wishes, there is no way I would have done what I have done. It is my fortune, she was my mother. Mom, I cannot thank you enough for being awesome.

I would like to dedicate the doctoral work to Late, Shri P. Sampath Kumar. Dad, I love you and will miss you forever. It is unfortunate you will not be there to see me as a Dr. But I know, deep inside you are above me and watching me every step of the way. You have always been kind and generous to people around you. Those who know you can speak for that. I will try my best to be like you.

v

\_\_\_\_\_

## TABLE OF CONTENTS

Acknowledgements ii	i
List of Tables	X
List of Figures xi	ii
Chapter I: Introduction	1
The Study	1
Tripartite Model of Matter	1
Common Research Methods for Exploring Chemistry Misconceptions	б
Study Design	7
Purpose of the Study	1
Research Questions	2
Assumptions13	3
Limitations14	4
Significance of the Study	б
Definitions	7
Organization of the Remaining Chapters in the Study18	8
Chapter II: Literature Review	9
Common Conceptual Difficulties on Chemical Equilibrium	0
Visualization and Microscopic, Macroscopic and Symbolic Representations	4
Relationship between Conceptual Errors and Visual Representations	9
Multimedia to Support Visualization in Chemistry Learning	0
Multimedia Based Theories	1

Sweller's Cognitive Load Theory (CLT)	32
Cognitive Theory of Multimedia Learning	35
Schnotz Integrated Model of Text and Picture Comprehension	
Advantages of using Visualization while Teaching Chemistry Concepts	44
Challenges and limiting factors	47
Computer Simulations and Chemical Equilibrium	48
Conceptual Change and Chemical Equilibrium	52
Conceptual change theories	57
Vosniadou's model	58
Posner's model	61
Disessa's p-prims model	62
Conceptual Framework for the Current Study	63
Chi's ontological shift model	63
Complex systems theory	67
Organization of the Remaining Chapters in the Study	70
Chapter III: Methodology	71
Chapter III: Methodology	71
Chapter III: Methodology	
	71
Purpose of the Study	71
Purpose of the Study Mixed Methods Design	71 72 75
Purpose of the Study Mixed Methods Design Research Questions	71 72 75 75
Purpose of the Study Mixed Methods Design Research Questions Research Hypotheses	71 72 75 75 75
Purpose of the Study Mixed Methods Design Research Questions Research Hypotheses Research Design	71 72 75 75 77 77
Purpose of the Study Mixed Methods Design Research Questions Research Hypotheses Research Design Participants	71 72 75 75 77 77 77
Purpose of the Study Mixed Methods Design Research Questions Research Hypotheses Research Design Participants Intervention	71 72 75 75 77 77 77 78 
Purpose of the Study Mixed Methods Design Research Questions Research Hypotheses Research Design Participants Intervention Sequence of Activities	71 72 75 75 77 77 77 78 79 
Purpose of the Study Mixed Methods Design Research Questions Research Hypotheses Research Design Participants Intervention Sequence of Activities Computer Simulations	71 72 75 75 77 77 78 79 

Data Analysis	90
Quantitative Data	
Qualitative Data	
Chapter IV: Data, Analysis and Results	97
Dissertation Study Results	97
Validity	
Face validity	
Construct Validity – Conditional Probability Analysis	
Reliability	
Frequency Analysis	
Pre-Quantitative/Qualitative data analysis	
Pre-Quantitative/Qualitative data analysis	
ANCOVA analysis	159
ANCOVA	159
ANCOVA assumptions	159
Results	
Simulation Notes-Sheet	164
Chapter V: Summary & Conclusions	167
Summary of Findings	167
Discussion	169
Research question 1	169
Research question 2	
Research question 3	
Research question 4	203
Connections to the Multimedia Framework	204
Implications and Ideas for Future Research	

## Appendices

APPENDIX A	207
APPENDIX B	211
APPENDIX C	222
APPENDIX D	
APPENDIX E	270
APPENDIX F	276
APPENDIX G	
	APPENDIX B APPENDIX C APPENDIX D APPENDIX E APPENDIX F.

REFERENCES	 

VITA
------

## LIST OF TABLES

Table 1, Sequence of simulations used in the study (* was not part of the pilot study)87
Table 2, Major sub-themes identified through the qualitative data in the current study95
Table 3, Demographics of participants who were part of the sample in the pilot phase of the dissertation study
Table 4, Conditional probability output generated using cross tab analysis of the pre-test data in SPSS representing the number of students assigned to the control group
Table 5, Conditional probability output generated using cross tab analysis of the pre-testdata in SPSS representing the number of students assigned to the experimentalgroup
Table 6, Conditional probability output generated using cross tab analysis of the post-test data in SPSS representing the number of students assigned to the control group104
Table 7, Conditional probability output generated using cross tab analysis of the post-testdata in SPSS representing the number of students assigned to theexperimental group
Table 8, SPSS output of the KR-20 analysis of the pre and post-test data for the control and experimental group         105
Table 9, Frequency analysis of common misconceptions held by students in the control(C) and experimental (E) group on the pre-test data
Table 10, Theoretical thematic analysis of control group's pre-qualitative data pertaining to item 3
Table 11, Theoretical thematic analysis of experimental group's pre-qualitative data         pertaining to item 3
Table 12, Theoretical thematic analysis of control and experimental group's pre-qualitative data pertaining to item 5
Table 13, Theoretical thematic analysis of control and experimental group's pre-qualitative data pertaining to item 8
Table 14, Theoretical thematic analysis of pre-qualitative data containing commonmisconceptions held by control and experimental group towards item 9118
Table 15, Frequency analysis of additional misconceptions held by students in the control (C) and experimental (E) group on the pre-test data. (NA = not applicable)
Table 16, Theoretical thematic analysis of pre-qualitative data containing additionalmisconceptions held by control and experimental group towards item 9121

Table 17, Theoretical thematic analysis of pre-qualitative data containing additional misconceptions held by control and experimental group towards item 11
Table 18, Frequency analysis of correct responses held by students in the control (C) andexperimental (E) group on the pre-test data125
Table 19: Thematic analysis of pre-qualitative data from the control group for item 3
Table 20, Frequency analysis of common misconceptions held by students in the control (C) and experimental (E) group on the post-test data
Table 21, Thematic analysis of common misconceptions held by students on the post-test towards item 3
Table 22, Frequency analysis of additional misconceptions held by students in the control (C) and experimental (E) group on the post-test data. ( $NA = not applicable$ )145
Table 23, Frequency analysis of correct responses held by students in the control (C) and experimental (E) group on the post-test data. (NA = not applicable)

## LIST OF FIGURES

Figure 1, Explanatory sequential intervention based design used with the experimental group during the dissertation study
Figure 2, Explanatory sequential intervention based design used with the control group during the dissertation study
Figure 3(a), Macroscopic view of a chemical equilibrium system at the start
Figure 3(b), Macroscopic view of a system that has attaind equilibrium. The figure also shows the microscopic view of the system using the lens option
Figure 4, A representative sample of the assessment tool developed for the study to assess qualitative data
Figure 5, Aspects of simulation appreciated by students164
Figure 6, Content aspect learned by students through the simulations166
Figure 7, Coding taxonomy developed to explain student's conceptual shift between ontological categories
Figure 8, Coding taxonomy demonstrating mental model held by student's in the experimental group during the pre-intervention phase
Figure 9, Coding taxonomy demonstrating mental model held by student's in the experimental group during the post-intervention phase
Figure 10, Graphical representation of the percentage of correct conception held by participants in the control and experimental groups during the pre and post phase203
Figure 11, Simulation of a system attaining chemical equilibrium
Figure 12, Simulation of a system attaining chemical equilibrium featuring concentration versus time graph
Figure 13, Simulation of a system attaining chemical equilibrium rate of a reaction in graphical form
Figure 14, Pulley experiment
Figure 15, Changing equilibrium conditions by addition of NO
Figure 16, Changing equilibrium condition by addition of NO, graphical representation of concentration change as a function of time

Figure 17, Changing equilibrium condition by addition of NO, graphical representation of rate of the forward and reverse reaction
Figure 18, Changing equilibrium conditions by decreasing volume of the system237
Figure 19, Changing equilibrium condition by decreasing volume, graphical representation of concentration change as a function of time
Figure 20, Changing equilibrium condition by volume change, graphical representation of rate of the forward and reverse reaction
Figure 21, Matrix representing the number of students assigned to a condition for each item based on the pre-test data for the experimental group
Figure 22, Matrix representing the number of students assigned to a condition for each item based on the post-test data for the experimental group
Figure 23, Matrix representing the number of students assigned to a condition for each item based on the pre-test data for the control group
Figure 24, Matrix representing the number of students assigned to a condition for each item based on the post-test data for the control group

#### **CHAPTER I. INTRODUCTION**

#### The Study

The mixed methods explanatory sequential study presented in this doctoral work aimed to explore student misconceptions or alternative conceptions towards chemical equilibrium concepts. Chemical equilibrium is an advanced topic typically encountered by students in the introductory second semester college level coursework or Advanced Placement coursework in high school. Numerous research studies have quantitatively and qualitatively explored student misconceptions towards this concept for more than three decades. While numerous research studies have explored student misconceptions toward chemical equilibrium, a relatively smaller number of those studies have explored the role of an intervention. The current experimental study aim to explore how students' mental model change as a result of intervention through visualization tool such as a simulation.

### **Tripartite Model of Matter**

Learning chemical equilibrium or even for that matter chemistry involves comprehending chemical phenomena at three levels: a)the macroscopic level of the system, b) microscopic level refers to the molecular, atomic and kinetic; and c) the symbolic level include symbols, equations, stoichiometry and mathematics, and making the coherent connections between the three levels (Johnstone, 1993). Macroscopic level describes phenomena that can be observed through the various senses. For instance, the different phases solid, liquid and gases can be observed through a visual cue or in special cases gases that are colorless can be sensed through smell. Symbolic level refers to the symbolic representations of atoms, molecules, and compounds used in writing chemical formulae and equations. As concrete learners, many students can easily observe chemical reactions occurring at the macroscopic level, but they have more difficulty making the transitions to microscopic and symbolic representations of chemical reactions, as these levels are invisible and abstract. While laboratory experiments tend to offer hands on experience, it does not immediately lend in to the idea of understanding particulate matter at the microscopic level. One of the primary reasons being experiments at the secondary or early undergraduate degree levels expect students to confirm results established prior to the commencement of the actual laboratory experiment. While, solving countless numerical problems might strengthen students' symbolic level understanding, it does not necessarily help them understand chemistry at the microscopic level. Qualitatively understanding a chemistry concept i.e., learning chemistry without all the mathematical calculations would be a viable option towards understanding chemistry at the microscopic level. In other words, performing countless mathematical calculations does not guarantee conceptual understanding of chemistry concepts.

According to Johnstone (1993), experts in chemistry have the ability to work well with all three levels and can easily transition between the three levels of representation, whereas students have difficulty making connections between the levels and may experience overload in their working memory. Chemistry instruction at the secondary or post-secondary levels typically focus on two of three levels, predominantly the macroscopic and the symbolic levels. Instruction at these two levels does not automatically render comprehension of the microscopic level among students, nor does it

allow students to transition between levels like chemists do (Nurrenbern & Pickering, 1987; Nakhleh 1993). Results of the these studies suggest that students with varying academic levels perform better on chemistry questions that are algorithmic/mathematical in nature, even towards questions that involve the sub microscopic level. Nurrenbern and Pickering (1985) demonstrated through their research study that many students were able to give correct numerical answers without applying content knowledge in solving chemistry problems. The study was co-operative effort between researchers at the University of Missouri, Kansas and University of Wisconsin, Stout. As part of routine examinations, students were requested to do both a traditional problem set on gas laws and a multiple choice test that had no mathematical content. Traditional problem set required students to use algorithmic strategies. Results of the study pointed out that, more than two thirds of students did not critically understand the behavior of gases, even though students showed proficiency at solving gas law problems. Gabel (1981), found that students were able to solve chemistry problems by application of algorithms that was not dependent on content knowledge requirement. According to Herron (1996), "algorithms are carefully developed procedures for getting right answers to exercises and routine tasks within problems with a minimum effort" (p. 64). Anamuah-Mensah (1986) suggested that instructors and teachers found it easier to teach chemistry problems through algorithms and formulas, thus ignoring the key aspect of conceptual knowledge. Through their review of research on chemistry problem solving, Gabel and Bunce (1991) found that students used what was referred to as a Rolodex approach, whereby they searched through memorized formulas until finding one where the units in the data matched the units in the problem. Solving chemistry problems in this manner focuses

students' attention on symbolic representations rather than developing a conceptual understanding that integrates symbolic and microscopic representations.

Learning difficulties towards conceptual understanding of chemistry can be partly attributed to this algorithmic method of learning. Phelps (1998) suggested that problem solving discontinuity is perpetuated in chemistry and other physical sciences because educators focus on an algebraic learning of chemistry, rather than supporting perpetual understanding. According to National Research Council (NRC) (1996), educators must probe for "students understanding, reasoning and utilization of knowledge" (p.82), so students learn concepts rather than learning exclusively problem solving. Pushkin (1998) listed four reasons to describe the disparity between conceptual understanding and algorithmic approach towards solving chemistry problems. They are a) students enrolled in general chemistry tend to follow a set of procedures and rules in solving problems, b) students display dualistic behavior – either act as repositories of knowledge, accepting information their instructors tell them without questioning it or accept their instructors perspective only under testing conditions, c) novice learners are subject to science curriculum and pedagogy that discourage critical and conceptual thinking and finally d) instructors who teach such classes also place more value on algorithmic learning than on conceptual learning, leaving the learners with the impression that science is "math in disguise" (p. 809). This aspect of algorithmic application of concepts towards solving chemical equilibrium problems will be one of the ideas explored in the study.

The concept of chemical equilibrium is a pivotal yet complex concept in chemistry. It is considered to be one of the most difficult topics in chemistry by students across classrooms (Treagust, Tyson, & Bucat, 1999, Quilez, 2004). Research studies

examining students' misconceptions or alternative conceptions about the concept of chemical equilibrium have been underway since the 1960s (Treagust, Tyson, & Bucat, 1999). Articles continue to be published on the topic of chemical equilibrium misconceptions among students and teachers even to the current day. The concept of chemical equilibrium is known to students attending chemistry classes and for which they have a preconception. The preconception of *equilibrium* stems from the idea used in everyday life, where equilibrium means equality of two sides, stability and static in nature (Schafer, 1984). While systems that reach chemical equilibrium may appear macroscopically stable and static, microscopically the system is dynamic not only because of molecular movement but also because the process of bond breakage and creation goes on. Gussarsky & Gorodetsky (1990) explained applying macroscopic qualities to the microscopic level leads to misconception towards understanding of chemical equilibrium.

Garnet & Hackling (1983) and Crosby (1987) pointed out that many students believe that even though equilibrium reactions are reversible they still go to completion, while other students think that the forward reaction goes to completion before the reverse reaction commences. In another instance, Gage (1986) found that students knew they had to compensate for changes in concentration of one reactant but could not correctly adjust all species involved in the reaction. Students often acted on the belief that the concentrations of reactants must equal the concentrations of products at equilibrium. In addition, these studies identified a general inability of students to distinguish between mass and concentration. Cheung (2009, 2004) have suggested while Le Chatelier's principle (LCP) is deceptively easy to apply to solve chemical equilibrium problems,

LCP is inadequate and can result in incorrect predictions about the effect of changes in concentration, volume, pressure or temperature on a chemical system at equilibrium. They concluded LCP is not a pre-requisite towards a deeper conceptual understanding of chemical equilibrium. Cheung (2009, 2004) suggested while teaching chemical equilibrium in classrooms teachers must not rely exclusively on LCP and should promote real learning by leaning towards the use of equilibrium law, concept of reaction quotient, and the simplified version of Van't Hoff equations.

## **Common Research Methods for Exploring Chemistry Misconceptions**

Research studies that have been underway to identify students chemical equilibrium alternative conceptions have employed a variety of methods towards assessing those misconceptions. The methods include a) conventional multiple choice tests, b) two tier multiple choice tests, c) clinical interviews, d) constrained word association and e) integrating the information obtained from multiple assessments (mixed methods – combination of quantitative and qualitative or multiple quantitative assessments). The conventional multiple choice test has been used in chemical equilibrium misconceptions research by (Johnstone 1977; Hackling & Garnett, 1985; Banerjee, 1991; Akkus, 2003; Canpolat et al, 2006, Bilgin et al, 2006; Atasoy, 2009), two tiered multiple choice tests has been used by (Treagust, 1988; Ozmen, 2008; Karpudewan, 2015). According to Treagust (1988), a two tiered multiple choice test more accurately reveals student misconceptions, as it minimizes the possibility students will receive credit for a correct answer, if they had chosen a wrong reason for a correct answer. The other more commonly used method towards assessing student misconception

has been clinical interviews. In the domain of chemistry clinical interview has been commonly employed to explore concepts of chemical equilibrium (Berquist andHeikkinen, 1990; Cheung, 2004; Voska, 1998; Williamson, 1992). An advantage to clinical interviews is that, it allows the researcher to probe for a deeper understanding of student misconceptions and thought process. A disadvantage with clinical interviews is it can be time consuming. Gorodetsky and Gussarsky (1986), employed constrained word associations to follow student learning about chemical equilibrium. Cheung (2009) employed think-aloud protocol to determine secondary school teachers' misconception towards chemical equilibrium. While many of the research studies mentioned above have identified student misconceptions towards chemical equilibrium, majority of the studies have focused on using one tier or two tier instruments for data collection. A relatively smaller fraction of studies have taken a qualitative approach to understand students' mental conception towards many of the chemical equilibrium concepts listed under (a-f).

## **Study Design**

The doctoral study uses a modified version of the advanced explanatory sequential design reported by Creswell (2014). The study is composed of two phases. Phase 1 involves the pilot study and phase 2 involves the research study. While the major purpose of the pilot study was to evaluate the quantitative instrument and the computer simulations, it also provided the opportunity to understand if students demonstrated conceptual gain towards chemical equilibrium concepts through the intervention. A single group pre (quantitative/qualitative)-intervention-post (quantitative/qualitative) format was adapted for the pilot study. A semi structured interview protocol was

employed to understand whether there was a change in students' thought process towards chemical equilibrium concepts following the use of the sequence of simulations. Analysis of covariance (ANCOVA) was conducted to answer the hypothesis that whether the posttest means, adjusted for pre-test scores, differ between the two groups. In addition students who participated in the pilot study were presented with a simulation notes worksheet. The purpose of the worksheet, is for students to convey a) what aspects of the simulation they liked the most and/or b) what aspects of the simulation they found confusing and/or c) what aspects of the simulation they like to be changed for future versions and/or d) what aspect of the simulation, they found helpful in terms of understanding the content etc. As a researcher, the worksheet allowed me to determine what information were students able to extract as they worked through each simulation. Each student may have a preference on what aspects they were able to extract through the simulation.

Student feedback during the pilot study was instrumental in making necessary corrections to the instrument and the simulations used in the research study. Construct validity was established through conditional probability analysis. Content validity was established through examination of the instrument by experts who have taught the topic of chemical equilibrium. The Kuder-Richardson 20 (K-R 20) analysis was performed to determine the reliability of the instrument. The K-R 20 was specifically used towards reliability analysis because, K-R 20 is a special form of Cronbach's alpha that is used when the quantitative instrument contains dichotomous data (right or wrong responses) and when the response data does not represent a continuous scale or cannot be ranked in any particular order.

Research studies that have explored the effect of interventions on students conceptual understanding of chemical equilibrium have identified several potential strategies to support conceptual learning, They are a) analogy models (Yildirim, Ayas, and Küçük, 2013, Raviolo and Garritz, 2009, Harrison, & De Jong, 2005, Stavy, 1991), b) mechanical mental models such as blocks, jig-saw (Doymus, 2008, Wilson, 1998, Cloonan, Nichol, & Hutchinson2011, Russell, 1998), c) co-operative learning (Stavy, 1991). Several researchers (Burke, Greenbowe and Windschitl, 1998, Sanger, Phelps, and Feinhold, 2000, Sanger and Greenbowe, 1997, Williamson & Abraham, 1995) have suggested that students who receive instruction that includes computer animations of chemical processes at the molecular level are better able to answer conceptual questions about the submicroscopic level. However, only Akaygun and Jones (2009) and Tang (2009) have conducted research studies examining student mental models about the dynamic nature of equilibrium change after viewing computer animations or simulations. While studies (Akaygun and Jones, 2009, Tang, 2009, Chiu, Chou and Liu, 2002 and Hameed, Hackling and Garnett, 1993) have looked in to understanding students' mental model they did not approach the concept of chemical equilibrium from a system's perspective, i.e., a change in a component of a system can influence other components contained in the system. For instance changing the volume of a system at equilibrium, affects the pressure of the system and how such a change affects the concentration of the species contained in the system.

The simulations presented in the study, were developed from a system perspective. The simulations present students with how concurrent changes occur in a system when an external change is made to the system. Students will be able to relate

changes happening at the particle level of the system to the graphical form containing information concentration and rate. Simulations were created using the SCRATCH platform (https://scratch.mit.edu/) developed at Massachusetts Institute of Technology (MIT). In each of the simulations presented in the study, audio and visual components were seamlessly merged. The Schnotz (2005) integrated text and picture comprehension model was used as the multimedia framework to guide the research study. The model lays its foundation on the philosophy taken by other models, i.e., comprehension is highly dependent on what kind of information is presented and how it is presented. The model proposes that only one mental model is constructed that integrates information from different sources right from the start. Another major contrast between the Schnotz model and cognitive structure based multimedia learning theories is, the Schnotz model assumes that pictorial information can not only be sensed through visual modality, but can also be conveyed by other sensory modalities such as sound images. This was visible during the post interviews in the pilot and research study. The graphs accompanying each simulation was unanimously voted as one of the best source of visual information by all participants. When inquired, does the audio played a significant role towards their change of answer choices, while some students suggested the graphical form superseded the audio component, others suggested the audio helped them to under the graphs better.

Rieber, (1990), suggested that effectiveness of animations can only be reaped if a) content and animation should be properly integrated, i.e., animation/simulation should be coincident with the content b) students must be provided with clear instruction and enough cues and c) interactivity and dynamics are two most important feature of animations. Tversky, Morrison and Betrancourt, (2002), suggested that successful

animations were found to have major characteristics a) animation must be readily perceived and comprehended and b) conceptual change to be conveyed must have been apparent from the animation. Research studies also indicate that effectiveness of visually enhanced instruction could be increased by using attention gaining tools, additional practice (Rieber, 1990) and explicit reasoning (Russell and Kozma, 2005). Burke, Greenbowe and Windschitl (1998), suggested effective instructional animation/simulation sequence must represent a) accurate chemistry content b) option to include text or audio narration c) panel with pause, forward and reverse control buttons d) interactivity, decision making, prediction for active learning e) appropriate assessment and feedback and f) includes misconception reported in the literature. Except for option e (appropriate assessment and feedback) all options were integrated in to the simulation design. The assessment was conducted externally through the chemical equilibrium misconceptions test (CEMT).

## **Purpose of the Study**

The purpose of this study was to evaluate the effectiveness of visualization tools such as simulations towards conceptual understanding of chemical equilibrium at the particulate level (microscopic) by students' at the post-secondary level. While research studies have explored effectiveness of low-tech instructional strategies such as analogies, jigsaw, co-operative learning, and using modeling blocks, few studies have explored the power of technology tools in learning homogeneous dynamic equilibrium. The study also sought to understand if students participated in the study held common misconceptions reported in the literature or in addition have students developed newer misconceptions

and what thought process guide a student to seek a particular answer choice on the quantitative instrument. The quantitative instrument used in the study was developed to reflect common misconceptions reported in the literature, along with a correct answer.

## **Research Questions**

The objective of the study is to investigate the following research questions

- a) What are students' conceptual understandings of chemical equilibrium before interacting with the simulations?
- b) What key characteristics of students' mental model regarding chemical equilibrium concepts can be extracted from student writings, drawings and oral explanation before viewing simulations?
- c) What evidence is observed to suggest changes in students' mental models on chemical equilibrium after they use the chemical equilibrium simulations?
- d) What are students' conceptions of chemical equilibrium after interacting with the simulations?

## Assumptions

The following assumptions guided the doctoral study:

- a) The student sample is representative of students who were enrolled in the four sections of the universities second semester introductory general chemistry courses.
- b) The topic of chemical equilibrium presented to students in the classroom through instruction is representative of the topic found in university general chemistry. This assumption allows the opportunity for the chemical equilibrium misconceptions test (CEMT), if established as reliable and valid, to be used in general chemistry classes at other universities.
- c) The qualitative interviews provides a valid and representative sample of student thought process about concepts, and transcripts extracted from student interviews represent authentic beliefs.
- d) The profile constructed from each student interview in the study represent actual concepts possessed by each student.

#### Limitations

- a) The study only explored student misconceptions towards a smaller fraction of chemical equilibrium concepts. Hence, the output of the study cannot be used to infer conceptions or misconceptions students may possess about other chemical equilibrium or chemistry concepts.
- b) Time was a major limiting factor in the study. This includes the time it took to recruit students to meet the necessary sample size for both the pilot and the research study, and the time a participant was willing to invest towards the study. Most participants spent about 90-120 minutes of their time to complete their portion of the study. If given more time to interact with each participant, greater detail from interviews might have been collected to richly portray participants' complex understandings of chemical equilibrium. As it was, the detail collected from participant interviews provided sufficient evidence to illustrate key scientific understandings developed through interacting with after students completed the simulation intervention.
- c) Limitations associated with interpreting qualitative interview include a) how the questions are cued was there inadvertent prompting, b) student response may be altered because of the presence of the researcher, c) concept modification during the course of the interview, d) the level of student conviction towards their responses, i.e. the student might have chosen a different reason to support their answer choice if asked to write their reason, rather than being asked to explain their reason orally when interviewed.

d) The simulations were developed by the researcher, and therefore depict the researcher's views and perspectives of chemical equilibrium. Student feedback was obtained during the pilot phase of the study, to make necessary corrections for clarity, to ensure simulations also depict aspects of a student's view.

#### Significance of the study

- a) The key significance of the current study is based on a system's approach towards chemical equilibrium using visual technology. While numerous research studies reported above have identified common chemical equilibrium misconceptions among students, none of the studies explored chemical equilibrium from a system's perspective.
- b) Currently there are no visualizations such as simulation or animation available that depicts the macroscopic view of a chemical system approaching equilibrium. The simulations contained in this study represent a chemical reaction at the particle level along with graphs that can allow students to relate the information contained in the graph to the reaction progress. The simulations also allow students to interact with the system.
- c) The simulations developed contain both audio and visual component to it. This allows the simulations to cater to students who are either visual or auditory learners or both.
- d) Another significance of the current study is the use of mixed methods approach to understand students' mental models. While numerous studies have explored students' conceptual difficulties towards chemical equilibrium, majority of those studies have used a quantitative approach and hence did not account for how students think while solving chemical equilibrium problems.

### Definitions

The following terms have been used throughout the study.

<u>Computer animation:</u> Computer animation is defined as a multimedia presentation that is rich in graphics and sound (Oakes & Rengarajan, 2002).

<u>Computer simulation</u>: Simulation as an interactive computer program that re- creates a specific model to enable learners to understand the phenomena through their interactions and explorations with the model (Oakes & Rengarajan, 2002).

<u>Dynamic equilibrium</u>: the condition in which a forward and reverse reactions are occurring simultaneously at equal rates (Atkins & Jones, 1997)

<u>Equilibrium constant:</u> In a reversible reaction, equilibrium constant (K) is the ratio of concentration of products over the concentration of reactants (Atkins & Jones, 1997) <u>Instructional technology:</u> Instructional Technology is the theory and practice of design, development, utilization, management, and evaluation of processes and resources for learning (Seels & Richey, 1994).

<u>Le Chatelier's principle:</u> A general principle that helps predict how the composition of a reaction mixture at equilibrium will change when the conditions are changed. This principle may be stated as, when a stress is applied to a system in dynamic equilibrium, the equilibrium tends to adjust to minimize the effect of the stress (Atkins & Jones, 1997).

<u>Molar concentration</u>: Expressed as a ratio of the number of moles of solute over the total volume of the solution in liters (Atkins & Jones, 1997)

<u>Reaction rate:</u> It is the speed at which a chemical reaction. Rate of reversible reaction can be expressed in terms of products which is formed in a unit of time or in terms or reactants which is consumed over a period of time (Atkins & Jones, 1997) <u>Reliability:</u> The extent to which results from a study are consistent over time and depicts an accurate representation of the population under study. If the results of a particular study can be reproduced under similar methodology, then the instrument used to obtain the results is considered reliable (Joppe, 2000).

# Organization of the remaining chapters in the study

The dissertation consists of five total chapters. Chapter 1 provided the background of the problem, context of the study, research questions, significance and limitations of the study. Chapter 2 provides a literature review on the tripartite model of matter, conceptual change approach towards chemical equilibrium, visualization and conceptual understanding, theoretical and multimedia framework used in the current study. Chapter 3 provides information about the research methodology, study design, quantitative instrument and the nature of data analysis. Chapter 4 provides brief analysis of results from pilot analysis, followed by analysis of data from the research study. Chapter 5 summarizes the findings from the research study along with implications recommendations for future research.

### **CHAPTER II. LITERATURE REVIEW**

Within the domain of chemistry, surveys have revealed that the topics of chemical equilibrium, the mole, oxidation-reduction and reaction stoichiometry give learners most difficulty; of these topics chemical equilibrium was rated as the most difficult for students to comprehend (Finley. 1982). Chemical equilibrium is an important concept which underlies much of high school and post-secondary level chemistry. In the paragraphs to follow we will closely examine key research studies that have been conducted over the last three decades regarding chemical equilibrium misconceptions. The scope of the literature review section would be to summarize 1) challenges of translation among the three levels of representation in chemistry, (2) resulting misconceptions students have in learning chemical equilibrium, (3) making the abstract concrete for learners through (a) graphics, diagrams in textbooks, (b) technology applications to create visualizations, and research on the power of these visualizations in learning; (4) constructing understanding in science, and in using models; (5) theories of learning through modeling. The proportion of articles exploring and assessing misconceptions outnumbered articles containing research studying intervention strategies and how such intervention had an effect on minimizing or eliminating misconceptions. The scope of this literature review encompasses a survey of students misconceptions on chemical equilibrium, difficulties navigating the three representations of chemistry in learning chemical equilibrium, support of technology in the form of animations and simulations to support learning in science, in general, and ...summarize methodologies and key findings used in the study and the rationale to engage in the current study to

understand and evaluate the role of instructional technology towards students' conceptual understanding of chemical equilibrium.

### **Common Conceptual Difficulties on Chemical Equilibrium**

The study by Hackling and Garnett (1985) is one of the earliest works on exploring students' misconceptions towards chemical equilibrium. They surveyed 12 secondary advanced chemistry students in a secondary school in Western Australia. The misconceptions were categorized in groups such as a) approach to equilibrium – when a reaction has begun and the system is approaching equilibrium b) characteristics of chemical equilibrium c) changing equilibrium conditions d) initial effects on rates of reaction e) rates of reactions when equilibrium is re-established f) effect on equilibrium constant and g) effect of catalyst. This study by Hackling and Garnett (1985) opened up the doors to areas of research focusing on students' conceptual misunderstanding towards chemical equilibrium.

In a study immediately preceding the study by Hackling and Garnett (1985), Gorodetsky and Gussarsky (1986) evaluated student misconception towards equilibrium using a three phase testing methods. The three phases was comprised of a) knowledge test b) misconception distractor test and c) cognitive structure mapping. The study also targeted similar areas of misconception studied by Hackling and Garnett (1985). The cognitive mapping structure consist of a procedure known as free sorting, were students would group concepts they think go together in groups. The cognitive structure mapping aims to attempt to reveal the conceptual connections that have evolved during a learning

process. Participants in the study were 12<sup>th</sup> grade high school students. Participants belonged to two groups. Group I was studying chemistry at a level that included topics such as nature of chemical equilibrium, quantitative aspects, meaning of Keq, factors affecting chemical equilibrium etc. Group II was studying topics studied by Group I, but they also studied chemical equilibrium in acids and bases, solubility and solubility product. Results of the study pointed out that students' performance on the misconception tests as poorer than on school tests. It was also found that low achievements on the misconception test was reflected in the latent categories of the free sorting of the appropriate group.

In a study by Berquist and Heikkinen (1990), student ideas regarding chemical equilibrium was explored from a qualitative perspective. The researchers interviewed students to find out what major misconceptions they carried regarding chemical equilibrium. The areas they identified students carried misconceptions are a) confusion over concentration versus amount b) appearance and disappearance of materials c) misuse of volume and d) confusion over gas behavior. As part of the instructional implications, the authors of the study suggested that since most general chemistry students had little or no conscious interaction with systems at equilibrium, it is hard to imagine that prior informal experiences could have shaped such misconceptions. They also added that such misconceptions could also be due to instruction that emphasis correct concepts without highlighting common conceptual errors experienced by students. They recommended that it would therefore be important to have a critical look at the instructional methods and materials in general chemistry courses.

Another major study concerning chemical equilibrium misconceptions was by Banerjee (1991). Participants of the study included 162 undergraduate students and 69 school teachers. A 21 item diagnostic test on chemical equilibrium was developed. The test consisted of seven multiple choice and eight short answer items on conceptual understanding, three items on problems solving and three items on applications to daily life. Analysis of the responses reveal widespread misconceptions among both students and teachers in areas related to the prediction of equilibrium conditions, rate and equilibrium, applying equilibrium principles to daily life, and to acid-base and ionic solutions in water. From the comparative study of the responses given by students and teachers reveals that the extent of misconceptions is equally high among both groups. The author concluded the possibility is that teachers might have developed these misconceptions during their days as a student. The misconceptions are retained, despite professional experience over the years.

Huddle and Pillay (1996) studied student misconceptions towards chemical equilibrium at the University of Witwatersrand. The study group consisted of students who were enrolled in a) Chemistry I class for engineering students b) Chemistry I class for students in medicine, pharmacy, nursing etc, c) Chemistry I class for chemistry majors and d) Chemistry I class for auxiliary students. The total participant count is 642. Students in all of the categories are presented two questions. The first question tasked students with making prediction based on the value of the equilibrium constant and calculate the amount of oxygen present at equilibrium. The chemical reaction can be found in Huddle and Pillay (1996). The second question expected students to calculate the concentrations of carbon dioxide, carbon monoxide, numeric value of equilibrium

constant and make predictions about the value of the equilibrium constant. It's been well reported in the literature prior to this study, that students often equate equilibrium to equal. Researchers of the study noticed, students cannot distinguish between rate and extent of a reaction.

Tyson and Treagust (1999) studied the complexity of teaching and learning chemical equilibrium, the researchers used a two tier test. One of the tier is composed of the actual choices for an answer and tier two consist of the reasoning. Only when both the multiple-choice answer and the reasoning response in both tiers were correct was the response, deemed to have answered correctly. The study revealed three issues; a) analysis of responses in the reason section of the two-tier test indicated that students used multiple explanations when predicting the effect of changing equilibrium conditions, b) use and interpretation of language emerged as a critical issue in the teaching and learning the topic of chemical equilibrium, c) highly sophisticated nature of the content of this topic was found to have important implication for its teaching.

Osthues (2005) investigated misconceptions among high school students who were enrolled in an advanced chemistry class around schools in Munster, Germany. All students who participated in the study were presented with a questionnaire containing multiple choice problems relating to common chemical equilibrium misconceptions. The researcher was also interested in finding out whether there was any correlation between chemical equilibrium misconceptions and mathematics knowledge, because research studies have revealed students misconceptions about chemical equilibrium have been related to student's lack of comprehension in mathematics.

#### Visualization and Microscopic, Macroscopic and Symbolic Representations

Learning chemistry involves comprehending chemical phenomena at three levels: a) macroscopic level of the system, b) microscopic level refers to the molecular, atomic and kinetic; and c) the symbolic level include symbols, equations, stoichiometry and mathematics, and making the coherent connections between the three levels (Johnstone, 1993). Macroscopic level describes phenomena that can be observed through the various senses. For instance, the different phases solid, liquid and gases can be observed through a visual cue or in special cases gases that are colorless can be sensed through smell. Symbolic level refers to the symbolic representations of atoms, molecules, and compounds used in writing chemical formulae and equations (Johnstone, 1993). According to Nakleh and Krajcik (1994), students construct most of the understanding of chemistry from a macroscopic perspective and fail to relate the macroscopic representations to symbolic and microscopic representations. According to Buckley and Boulter (2000), the purpose of models and modeling in science education is to assist with understanding scientific content, thinking logically and creatively, constructing knowledge structures, developing problem solving skills and making evaluations during the course of scientific learning. If models can be interactive, it can provide a bridge between science education and technology (Gilbert et al, 2000). According to Kress et al (2001) visualization is more than a tool for learning, because it enables learners to make meanings or express their ideas which cannot be readily done so through a verbal representation alone. Kozma and Russell (2005) suggested, the meaning of a representation is not embedded in the representation itself, but is assigned to the representation through its use in practice.

Bowden (1998) and Kozma and Russell (1997) suggested the concept of representational competence. According to representational competence, learners must be able to transform representations in one form to an equivalent representation in another form. Kozma and Russell (1997) in a study explored expert chemists' and novice students' understanding of various forms of representation and their ability to transform between one form of representation to another. Study results suggest that experts were able to switch between representations with much ease compared to novices. According to deJong et al (1998), representations in science and mathematics can be used as a means to conceive abstract concepts and be able to solve problems. In sharp contrast to single representations such as a stand along diagram, multiple representations in the case of chemistry consisting of formula and diagram can support deeper development, when learners can combine multiple pieces of information to develop a fruitful insight (Berthold and Renkl, 2009). While multiple representations add more value compared to single representations, theories on learning with multiple representations suggests, learners who are using multiple representations must be able to understand each representation on its own. Learners must be able to understand which parts of the domain are represented through the representations (Ainsworth 2006, 2008; Moreno and Duran, 2004; Seufert 2003, Van der Meij, 2007).

In addition to relating one representation to the other, learners must also be able to interpret the similarities (Ainsworth, 2008 & van der Meij, 2007). In an experimental study Corradi et al (2012) examined how use of multiple external representations (MER) lead to increased conceptual understanding among learners with low and high prior knowledge about the content. Students were assessed for their nominal and functional

literacy. Nominal literacy is used to assess participants' recognition of chemical concepts. Functional literacy is used to assess participants' ability to describe concepts. Learners were assigned to four groups each presented with a different form of external representation. Group1 received only information through textual form, group 2 received information through a combination of symbolic and textual form, group 3 received information through a combination of text and image and group 4 received information through a combination of text, and image and group 4 received information through a combination of text, image and symbol. The results of the study concluded that students with low prior knowledge benefited from using aids and tool to increase their conceptual understanding, whereas learners with high prior knowledge gained no benefits from the use of aids or tool. The authors suggested when teaching learners with low prior knowledge, instruction should contain text and symbolic representation guided by instructional aids such as prompts or note taking. After learners have reached a certain level of understanding, microscopic representation can be added to instruction to optimize learning.

Gobert and Clement (1999) suggested that diagrams have more than illustrative purpose, as it can also serve the purpose of model construction and reasoning. The visual impact of diagrams can enhance the development of mental models and leads to more connectedness in learning. Stylianidou et al (2002) examined students' interpretation of diagrams in science textbook exploring the topic of energy. The study concluded a visual representation of the topics on energy through diagrams was not trivial to students and teachers should spend time assessing the meaning of the images with students. The study also revealed that text when combined with diagrams provided learning gains. Matthewson (1999) suggested, in chemistry because of the significance in visualizing

molecular structures, much of the focus has been dedicated on how students perceive three dimensional molecular structures from two dimensional representations. Matthewson (1999) suggested that while visualization is necessary to perceive three dimensional structures, it is not the only topic that requires visualization. Conceptual understanding of topics such as stoichiometry, chemical bonding and particle model each requires a different kind of visualization.

Harrison and Treagust (1996) studied how students in grade 8-10 viewed the atomic model and electron arrangement inside an atom. Students were presented with 6 diagrams of the atomic model with varying representation of electron cloud. While majority of students were able to eliminate model 6 (a ball model), because the model represented a point mass view. At the same time, many of students opted for model 2 (orbits model), which is also an incorrect version of the atomic model. Students' reasoning behind their choice for model 2 (orbits model) was it appeared distinct and concrete. The study results suggested that students' preference could inform teachers about students' prior conception when they start to learn advanced atomic models in which electrons do not follow specific orbits. The study also brought up the idea on how students' perceive the idea of electron cloud. Bar (1989), while investigating students' knowledge of the water cycle determined, students' viewed cloud as sponges in which droplets of water is embedded.

According to Gilbert (2008) students' difficulties understanding chemistry concepts can be attributed to the meta-visualization capability to understand and translate between various modes of representation, i.e., ability to acquire, monitor, integrate and extend learning that involve both internal and external representations. Internal representation

(mental models) refers to a real or fictional state of a phenomenon, usually built on the spot in response to a specific learning situation for which the learner has no available schemas to fit the phenomenon in order to deeply understand and reason about the phenomenon (Buciarelli & Cutica, 2012). On the other hand, external representation in science refer to graphics, diagrams, models, simulations, etc, typically used in learning (Buciarelli & Cutica, 2012). This idea expands on Johnstone's (1993) model of the three levels of representation needed to understand chemistry. According to Gilbert (2005), meta-visualization involves demonstration of five key capabilities in a wide range of context. They are a) Understanding the conventions of representation, b) Capacity to translate between modes and sub modes and between various levels of representation through which it can be represented, c) Ability to construct representation in any mode and sub-mode for a given purpose, d) Ability to use visualization to construct predictions of a particular behavior in respect of a given model and e) Ability to solve new problems by constructing analogies to already used visualizations.

External representations can also be presented through dynamic or multimedia modes. A dynamic mode usually presents abstract phenomenon in the form of animations or simulations and a multimedia mode typically contains a combination of external representations. The authors hence put forth a list of guidelines for teaching and learning with external representations. They are 1) cognizant of learning theories towards use of external representations, 2) understand key factors that affect students' ability to visualize external representation, 3) conceptual knowledge addressed by the external representation must be made explicit to students, 4) ensure knowledge of the visual language and convention used in the external representation, 5) students must be aware of the

limitations behind an external representation, 6) instructors must foster a multiple external representation approach, 7) empower students with necessary skills needed to process external representations, 8) developing students' metacognitive skills and 9) use of learner generated external representations.

### **Relationship between Conceptual Errors and Visual Representations**

According to Ben-Zvi et al (1987) and Krajcik (1991), alternate conceptions about chemical concepts arise from a) representing chemical concepts only at the macroscopic level rather than in combination with microscopic and symbolic level b) comprehending chemical concepts at the macroscopic level through surface features and c) interpreting chemical reactions as a static processes. Ben-Zvi et al (1987) reported that despite substantial instruction, students in the study viewed formulas were merely abbreviations for names rather than a composition or a structure.

Keig and Ruba (1993) claimed that translating between representations is an information processing task and requires the knowledge of an underlying concept. Possessing conceptual knowledge allows learners to interpret the information contained in the incoming representation and manipulate it construct the target representation. According to Wu et al (2001), chemical representations are conceptual constructs that require a combination of cognitive linkage between the conceptual components that centers around content knowledge of underlying concepts and visual components that allows a learner to decode and interpret the symbols and conventions. To justify the claim proposed by Wu et al (2001), Paivio (1986) proposed that if there is a linkage between the cognitive and visual component, conceptual understanding can be increased by

allowing the learners to compare to multiple representation of a single object. Paivio (1986) through an empirical study observed that students viewed a water molecule (H<sub>2</sub>O) to contain H<sub>2</sub> gas. To justify the above claim Paivio (1986) suggested, presenting students with multiple representations of water molecule through ball and stick model, structural formulas, so students can have a better conceptual understanding

### Multimedia to Support Visualization in Chemistry Learning

As pointed above, one of the reason behind students' conceptual errors towards chemistry is, they hold a static model of chemical reactions, represent chemical reactions at the macroscopic level through surface features, rather than transitioning to a microscopic level to illustrate the dynamic nature of reactions. Jones and Berger (1995) through an empirical study examined student use of a multimedia chemistry instructional program used in an undergraduate chemistry course. Log files from a class of over 500 undergraduate students were examined to determine time spent on the software and student use of the software's media components. In addition to examining overall behavior profiles across the class, they examined variation within individual students, through use of sequence analysis. Their results point out that, use of videos and animations in combination were helpful to students experience properties of light, energy and molecules which would otherwise be difficult.

Schank and Kozma (2002) in an empirical study involving 42 high school students using the solubility curriculum module. Using ChemSense as a platform and the solubility module as the content, students created drawing and animations over a three week period. Students demonstrated greater representational competence and deeper understanding of geometrical aspects of chemical phenomena in their animations. Kozma and Russell (1997) developed "*Multimedia and Mental Models*" also known as 4M:Chem a multimedia software to enable chemistry instruction. The model was developed as a protocol and was never used on a production level. The 4M:Chem model of a chemical equilibrium process contains a video of the chemical reaction, an equation with symbols and formulas, an animation representing the molecular motion at the microscopic level and a graph representing the change in concentration. The idea behind the 4M:Chem model is for students to develop referential links between the various representations.

In summary, Wu and Shah (2004) suggested the following design principles are critical towards use of visualization to enhance conceptual understanding. They are a) providing multiple representations and descriptions, b) linking visual and conceptual ccomponents, c) presenting chemistry in its dynamic form, d) promoting transformation between 2D and 3D, and e) reduction in cognitive load.

### Multimedia based theories

In this section the various theoretical frameworks that have been used in the context of multimedia learning will be addressed. The following theories have had the greatest impact towards multimedia based learning. They are a) Sweller's cognitive load theory (CLT) (Sweller, 1994), b) Mayer's cognitive theory of multimedia learning (CTML) (Meyer, 2001), c) Integrative model of text and picture comprehension by Schnotz (Schnotz, 2005) and d) Van Merrienboer and Kester's four-component instructional design (Van Merrienboer & Kester, 2005).

# Sweller's Cognitive Load Theory (CLT)

Cognitive load theory (CLT, Sweller, 1994) sought to understand and integrate knowledge of human cognitive structures and instructional design principles. The cognitive load theory examined the working relationship between the working memory, long-term memory and sensory memory. According to Sweller (2003), learning has occurred when alteration occurs in long term memory. Long term memory is a cognitive structure that is a repository for knowledge. A human mind only recognizes information that is being transferred from the long term memory in to working memory.

If alteration of long term memory has to happen for learning to occurs, how can such a change happen to long term memory, as material is learned? What constitutes a schema? According to Sweller (2003), schemas are cognitive constructs that enable multiple elements of information to be categorized as a single element. According to Piaget (1928), a schema is both the category of knowledge as well as the process of acquiring it. When encountering new information or experience, new schemas are developed or existing schemas are modified. According to Bartlett (1932), schema is a network of abstract mental structures. As the complexity of a domain increases, the number of schemas that need be acquired increases. Looking through the multimedia lens, knowledge is held in a schematic form in long term memory visually (picture) or verbally (written or spoken). Acquired schema can be processed consciously or automatically. For instance, a chemist solving a complex chemical equilibrium problem can process all the necessary schemas associated with the problem automatically. The reason being, the acquired schema has been practiced over long periods of time. To

enable a novice to become an expert, it would be important for them to consciously recognize the schemas necessary to solve a similar chemical equilibrium problem.

The ability to process information consciously or automatically requires interaction between the working memory and the long term memory mediated by the sensory memory (ears or eyes). What is a working memory? Similar to long term memory it is a cognitive structure, where incoming information is processed. While processing new information, working memory is constrained by two limitations. According to Miller (1956) working memory can only accommodate a maximum of seven elements from the new information. While a maximum of seven elements can be accommodated at a time, only two to four elements can be combined, contrasted or manipulated. The second limitation being the duration for which the new information is processed. Peterson and Peterson (1959) reported that without rehearsal, all information contained in the working memory is lost within about 20 seconds.

According to Baddeley (1992), working memory was not treated as a single entity, but rather has a three-component system consisting of a central executive, a visuospatial sketchpad and a phonological loop. The purpose of the visuo-spatial sketchpad is to deal with two and three dimensional objects and the phonological loop's purpose is to deal with auditory materials such as speech.

Mayer (2001) suggested that if instruction is designed to make use of multiple processors, learning can be productive. The limitations of the working memory suggested above does not apply to information that has already been organized in to schemas in long-term memory and needs to be processed by the working memory. Hence, the working memory capacity cannot be a factor that distinguishes an expert from a novice; it

is how well the information is organized in to schemas in long-term memory. According to cognitive load theory (CLT), whether information is presented through multimedia, direct instruction or other forms of instruction, three categories of cognitive load must be recognized. They area a) extraneous b) intrinsic and c) germane cognitive load. Extraneous cognitive load occurs primarily when instructional design is inadequate and does not consider working memory limitations on schema construction and automation.

A number of researchers have developed principles to address the effect of extraneous cognitive load. For example, a) worked example principle (Cooper & Sweller, 1987) b) modality principle (Tindall et al, 1997) c) split attention principle (Sweller et al, 1990) d) redundancy principle (Chandler & Sweller, 1991) and f) expertise reversal effect principle (Kalyuga et al, 2003). According the worked example principle, when learners show increased efficiency with learning when solving problems that provide a solution to the problem. Reducing or eliminating the heavy demands on working memory and schema construction through the worked example reduced extraneous cognitive load.

The split attention principle, a student must channel his/her attention towards multiple sources of visual information, all of which are essential for understanding. Information coming in from all the sources must be coherently integrated before the information can be understood. The heavy load placed on working memory during mental integration leads to extraneous cognitive load. Through physical integration of multiple sources of information, extraneous load can be reduced

While the modality effect share commonalities with the split attention effect, extraneous cognitive load can be reduced by not physically integrating information from

multiple sources, but by presenting verbal information in spoken rather than written form. This allows for increased working memory capacity.

According to the redundancy effect, while multiple source of information is presented, one source of information is sufficient to allow understanding and learning and the rest of the sources reiterate the information from the first source through various forms. Extraneous cognitive load is reduced by eliminating redundant information rather than eliminating split attention or modality effect.

The expertise reversal effect occurs when information that is essential for novices becomes redundant for more expert learners. Intrinsic cognitive load is related to the complexity of the material being presented. If the material present contain higher degree of element interactivity, it leads to higher intrinsic cognitive load, because of higher load is placed on working memory capacity.

Effortful learning results in germane cognitive load. In other words germane cognitive load is healthy cognitive load that is necessary towards successful learning. In conclusion, according to the cognitive load theory whether direct instruction or instruction mediated through multimedia must be designed around working memory limitations and the role of extraneous and intrinsic cognitive loads.

# **Cognitive Theory of Multimedia Learning**

According to Cognitive Theory of Multimedia Learning (CTML), "individuals learn more deeply from words and pictures than from words alone" (Mayer, 2001, p.47). CTML is grounded on three foundational principles a) active processing of information b) dual channel processing and c) active processing. In addition to the above mentioned principles, CTML also defines five major cognitive processes that are essential in a multimedia learning environment. The cognitive processes occur in the working memory while processing new incoming information. The five cognitive processes are a) selection of relevant words b) selection of relevant images c) organizing information in the word form to create a verbal mental model d) organizing information in the picture form in to a pictorial mental model and e) integrating the verbal and pictorial model with each other and with prior knowledge to create a coherent model.

In the dual-channel assumption, the information processing system consists of an auditory channel processing information received in the verbal form and a visual channel processing information received in the pictorial form. According to Mayer (2004), the dual channel information processing system can be conceptualized in two ways. One way is based on the presentation mode and the other is based on the sensory model. While the presentation mode dedicates focus towards the nature of stimulus presented (picture, text, animation, sound etc.), the sensory mode dedicates focus on the stimulus as represented in the working memory. The CTML relies heavily on the sensory mode of information processing. While information is always received through one of the channels (verbal or auditory), learners may also be able to convert the representation for processing in the other channel.

In the limited capacity assumption, the working memory in the human cognitive system can only process limited amount of information in each channel under a given time frame. Through practice, learners can construct techniques for chunking elements contained in the information in to groups. Chunking allows for increased learning efficiency. As pointed out earlier in the cognitive load theory section, instruction must consider the limitations of working memory capacity.

In the active processing assumption, active cognitive processing is necessary to develop a coherent mental representation. Active cognitive processes include a) paying attention b) organizing information c) integrating newer information with existing information. If the key objective of active learning is construction of coherent mental models, it is worthwhile to understand ways through which knowledge can be structured. The knowledge structures include process, comparison, generalization, enumeration and classification. Process structures consist of explanations on how a particular system works. Comparison structures as the name implies compares two or more elements contained a matrix form. Generalization structure consists of a major element and a series of sub-ordinate elements branching from the major element. Enumeration structures consist of lists, with each list containing a list of elements. Classification structures consist of a hierarchy of sets and subsets. Comprehending a multimedia message requires a learner to construct one or more of the knowledge structures. The assumption that learner's develop a knowledge structure while comprehending a multimedia message leads to two key implications. They are a) presented material must be coherent – if the incoming material consists of isolated facts, learner's efforts to build a mental model or representation will be futile and b) the message should provide sufficient guidance, so the learner can learn how to build a coherent mental model.

According to CTML, the working memory is partitioned in to two parts. One part consists of raw material that comes in to the working memory from the sensory memory through visual and auditory channel. The other part of the working memory consists of

knowledge structures constructed in the working memory (pictorial and verbal model). In both parts there is a link between the two channels. The link suggests students may process verbal information in to pictorial information or vice versa.

While the two assumptions above suggest how information should be presented, the five cognitive processes mentioned above suggest how the presented information is processed by a learner. The cognitive processes do not follow a linear order. In other words, a learner may move from one process to the other in a random fashion.

Cognitive process occurring through selection of words or images depends on the nature of external representation or input. If the external representation or input is in the form of spoken words, the output is a mental representation of the words in the learner's verbal working memory. The learner must determine what aspect of the information is most relevant. The need to select only part of the information occurs because of limitations in the working memory capacity. If information is presented through pictorial representation, the output is a visual image base, i.e., a mental representation of the images in the learner's working memory. The process begins in the visual channel, but a learner might be able to convert a portion of it in the auditory channel. Similar to selection of words from incoming information, a learner must be able to assess and select relevant images that need to be processed in the working memory. Selected words or images are then converted in to verbal or pictorial model in the working memory. The key step in multimedia learning involves the construction of linkage between the pictorial and the verbal model. In light of the cognitive theory of multimedia learning (CTML), multimedia based instructions that are designed in light of how the human mind functions are more likely to lead to meaningful learning.

#### Schnotz Integrated Model of Text and Picture Comprehension

The Integrated Model of Text and Picture Comprehension (IMTPC, Schnotz, 2) shares many similarities with the two models already discussed, but offers specialization of sensory registers in learning through multimedia visualizations. The cognitive architecture of the model consists of working memory, sensory registers and long term memory In addition the model's architecture consists of a cognitive level and a perceptual level. The cognitive level consists of a verbal and pictorial channel and the perceptual level consists of multiple sensory channels. The role of the perceptual level is to transfer information from the stimulus to the working memory through sensory registers and the role of the cognitive level is to process information in the working memory and transfer it to the long term memory for later usage. Another major difference between CTML and the current model is, the former model assumes independent construction of a verbal mental model and pictorial model which then later have to be integrated. The current model proposes that only one mental model is constructed that integrates information from different sources right from the start. Another major contrast between the current model and CTML is the current model assumes that pictorial information can not only be sensed through visual modality, but can also be conveyed by other sensory modalities such as sound images. Based on empirical evidence the following positive effects have been derived from the use of auditory pictures.

# Coherence and Contiguity

Coherence refers to the condition under which words and pictures are semantically related and contiguity refers to the condition under which words and pictures are presented closely together in space or time. The coherence and contiguity aim to address the limitations of the working memory capacity. Temporal contiguity aims to reduce the limitations of the working memory capacity by presenting pictorial and semantically related auditory information simultaneously. Because information is presented through spoken text rather than written text and is semantically related to the pictorial information presented, pictorial and the auditory channels become active and process information simultaneously. This allows for the split attention effect commonly observed with written text associated with pictures. Spatial contiguity aims to reduce the visual search processes because pictures and the spoken text are closely related to each other. By reducing the visual search process, the cognitive load typically placed on the working memory is reduced.

# Modality

There are two outcomes arising from the modality effect. The first being the split attention effect discussed in the coherence and contiguity section above. Another aspect of the modality effect is the working memory capacity that is required for active cognitive processing. Mayer and Moreno (1999) in a study examined the effect of spoken versus written text in combination with pictures on learning gains. They found that students who learned through spoken text in tandem with pictures showed better learning gains. Since working memory has high decay rates, construction of propositions and mental models requires simultaneous availability of text and pictorial information.

# Sequencing

According to a study conducted by (Kulhavy et al , 1994), presenting pictorial information before text leads to better understanding According to the current model, a

text (spoken or written) does not entirely describe with enough detail to fit just one single picture or mental mode. If mental model construction occurs entirely through text processing, the model developed will differ to some extent from the picture that illustrates the subject matter. Hence there is an interference effect if the text is presented prior to picture presentation.

### Reading Ability and Prior Knowledge

In addition to the assumption that text and picture comprehension corresponds to alternate routes of constructing mental models and propositional representation, the model associates the role of prior knowledge. The auditory pictorial representation can assist learners who are poor readers. When learners have poor reading proficiency, the auditory channel loses its efficiency while the visual channel plays a dominant role. This prediction has been verified by empirical research findings in the work of Swanson and Cooney (1987), Levie and Lentz (1982). When learners encounter information towards which they have weaker prior knowledge, pictorial information can enhance mental model construction. On the flip side, students with higher level of prior knowledge tend to gain no additional advantage through pictorial representation.

# Redundancy (specific and general)

Specific redundancy effect occurs when pictorial representation is accompanied by both spoken and written text reinforcing identical information contained in the pictorial form. Specific redundancy effect is the direct result of multimedia designer's frequent attempt to tailor instruction to individual needs. Multimedia designers often combine spoken and written text along with pictures with the hope that learners have the option to choose their preferred sensory modality. The integrated model predicts that learners do not show any learning gains when they learn pictures associated with both spoken and written text, rather they only benefit when pictures are associated with spoken text. Mayer (2001) in a study examining the specific redundancy effect suggested learners showed lower performance when learning content through both spoken and written text associated with a picture in comparison to learners who learned similar material through spoken text and pictures. The difference in learning gains is attributed to the split attention dedicated between spoken and written text when they are used in combination with pictures.

General redundancy effect is commonly observed when learners with high prior knowledge are exposed to material containing both picture and auditory text. Learners with high prior knowledge do not make use of the additional source of information and often exhaust their working memory capacity through split attention. To understand the role of incorporating learner experience into the design of multimedia instruction, Kalyuga et al (2000) conduced a research study. The research study consisted of two separate experiments. Sixty trade apprentices from two major Australian manufacturing companies' participated experiment 1. In experiment 1, inexperienced trade apprentices were allotted to one of the four group; a) a diagram with visual text, b) a diagram with auditory text, c) a diagram with both visual and auditory text and d) diagram only. In experiment 2, 38 apprentices from experiment 1 were assigned to two groups; a) diagram only and b) diagram with audio text. In experiment 2, the diagram only group was compared with the audio-text group after an additional training session. Results from experiment 1 pointed out that auditory presentation of text proved superior to a visual

only presentation but not when the text was presented in both auditory and visual forms. The diagram only format was the least intelligible to the apprentices. The results from experiment 2 were reverse to those of experiment 1. The diagram only group outperformed the audio-text group. The authors attributed the reversal in results is due to the knowledge and experience gained by apprentices between experiment 1 and 2.

# Structure Mapping

According to the integrated model, visualizations can only be beneficial if they are presented to learners in a task appropriate manner. The assumption is supported by empirical research findings reported by Schnotz and Bannert (2003). In their study Schnotz and Bannert examined the role of informationally equivalent pictures associated with text on learners understanding of the material. They found that pictures enhanced comprehension only if the content was visualized in a task appropriate manner.

Deep versus Superficial Processing.

When pictures and text are presented in a combined form, one form can also replace the other to a certain extent. If picture is added to a material containing text, and if identical amount of mental effort is invested by a learner, textual information can become less insignificant due to concurrent existence of pictorial information. Hence, the text will be processed less deeply resulting in the use of a lower memory towards text information than if the text information had been presented without pictures.

# **Cognitive Economy**

When multiple representations about a single topic are processed by the working memory, the additional benefit for comprehension is outweighed by the additional

cognitive costs. Learners choose cognitive economy when the benefits associated with processing additional information are lower.

In conclusion, similar to the cognitive theory of multimedia learning, the integrated model rests its assumption on the philosophy that multimedia learning can only be successful when the design principles are guided by sufficient understanding of human perceptions and cognitive processing systems. Positive and negative effects presented in the section must be considered while designing multimedia instruction. The Schnotz integrated multimedia framework will be guiding the work.

### Advantages of Using Visualization While Teaching Chemistry Concepts

Chemistry is often regarded as one of the difficult subjects, a notion that often repels learners from continuing with studies in chemistry. However, chemistry is one of the important branches of science that allow learners to understand how and why things work the way they should. Because chemistry topics are generally related to or based on the structure of matter, chemistry proves a difficult subject for many students. Chemistry curricula commonly incorporate many abstract concepts, which are central to further learning in both chemistry and other sciences (Taber, 2002). Learning of abstract concepts is essential to understanding advanced concepts and theories. If underpinning foundational abstract concepts are not understood, it leads to conceptual difficulty (Zoller, 1990; Nakleh, 1992). Learning chemistry requires students to understand representations in macroscopic, symbolic, and microscopic levels. However, students often have difficulty understanding abstract phenomena like behaviors of atoms and

molecules. This is because subatomic particles cannot be viewed or experienced directly and hence the concepts are abstract. Meanwhile, many of these students' intellectual development is at the concrete operational stage (Herron, 1975; Goodstein & Howe, 1978a, 1978b; Abraham, Williamson, & Westbrook, 1994). As a result, students need some concrete analogies, which can be felt, touched, or visualized, to aid them in learning concepts using atoms and molecules. The ability to visualize molecular behavior and think at the atomic and molecular level is essential for understanding chemistry concepts. Therefore, helping students visualize particulate phenomena is an important goal of chemical education.

Effective use of technology not only makes the process of teaching and learning productive, but also can provide teaches with the tool to bridge the gap between conventional learning and modern educational requirements for the overall development of the learner (Gupta et al, 2012). Sanger (2006, 2009) reviewed a series of research studies on the use of computer animations in chemistry. These studies showed that (a) students improved their conceptual understanding and performed better in exams after viewing computer animations, (b) students who viewed computer animations at the microscopic level had fewer misconceptions than students who only received traditional instruction, and (c) compared to students who only viewed static pictures, students who were exposed to computer animations understood conceptions at the microscopic, macroscopic and symbolic levels more completely.

Yezierski and Birk (2006) investigated the effectiveness of computer animations in changing students' misconceptions about the particulate nature of matter, especially those related to phases and phase changes. The results indicated that animations at the

atomic and molecular level aided the students in forming better mental models and to develop conceptual understanding of particle properties and behaviors. Visual technology also allows chemistry experiments to be performed electronically when i) a school does not have supply of chemicals or resources ii) when school is located in a low Socio Economic Status (SES) areas iii) lack of infra-structure to conduct experiments safely iv) allow students to repeat experiments as many times as they would like without having to worry about starting over or generating chemical waste v) they can also share their work through the world wide web with other schools across the world. The process of conceptual change is an ongoing challenge in science education, particularly among members of the chemical education community. Computer simulations have demonstrated the potential to facilitate this process by highlighting students' misconceptions and presenting plausible scientific conceptions. For instance, using computerized interactive laboratory simulations, learners can confront their beliefs by working with real data, experiencing discrepant events preselected by the program, or forming and testing multiple hypotheses of their own (Gorsky and Finegold 1992; Tao and Gunstone 1999; Trundle and Bell 2005).

In summary, computer simulations and animations in chemistry help student connect representations of chemical phenomena in the macroscopic, symbolic, and microscopic levels. Such visualization also help students build more correct mental models of chemical concepts and develop conceptual understanding.

#### **Challenges and Limiting Factors**

While there are proponents who support the use of computer simulations/animations and other dynamic visual media in to instruction, research studies conducted by other researchers oppose this view. For instance, (Lowe 2003) suggested that animations can confront learners with additional and qualitatively different information processing demands than static visuals. Lewalter (2003), suggested that while transitory nature of animations may reduce the load due to cognitive processing through support of mental model construction, the transitory nature in itself may cause higher cognitive load since learners have less control over their cognitive processing. Mayer and Moreno (1998), suggested based on their research study that when students observe different types of representation through visualization, it may cause them to experience difficulties in processing the information because of the split attention effect. According to Rieber (1991) if animations are not closely related to the contents, or are poorly designed, they have little or no effect on student understanding of the concept. If animations are too easy, they are not effective, or the effect cannot be detected when comparing to the control groups, because of the ceiling effects. If animations are too complex, and students do not have enough time to explore them, they will feel frustrated and give up. The following aspects could be challenging or limiting a) whether simulations or animations specific to a particular topic is already available? b) whether such visualizations are available for use at free of cost or requires expensive subscription, c) does the visualization depict accurate content?, d) are there enough such devices available to accommodate an entire class?, e) do devices (computer or similar electronics) meet the minimum hardware requirements?, f) many chemistry simulations available in

the market or through the worldwide web are not compatible with mobile devices or devices that are not capable of running Java® or Adobe Flash® platforms and g) above all, how the visualizations are used contributes a lot towards its efficiency.

### **Computer Simulations and Chemical Equilibrium**

Analogy and its derivatives, remains one of the sought out strategy reported in the literature. While effect of computer visualizations on students understanding of chemistry at the particle level has been extensively addressed, use of computer simulations and animations to teach chemical equilibrium remains very limited and far from a few. After an exhaustive literature search and review, it can be asserted, the study by Hameed, Hackling and Garnett (1993) till date remains the only study that has examined all chemical equilibrium misconceptions reported by Hackling and Garnett (1985). The study was based on the conceptual change model proposed by Posner, Strike, Hewson and Gertzog (1982). According to the Posner et al (1982), the scientific conception must also be intelligible, plausible, and fruitful for successful conceptual change to occur. Intelligible means that the new conception must be clear enough to make sense to the learner. Plausible means the new conception must be seen as plausibly true. Fruitful means the new conception must appear potentially productive to the learner for solving current problems.

The study examined the use of computer assisted instruction (CAI). The CAI package was developed using BASIC programming language and were used on microcomputers. The article does not provide details on what components made up the program or how the components were organized or even a representative figure of the

program. The use of CAI package was guided by five principles a) presentation of phenomenon b) prediction c) simulation d) explanation and feedback and e) application. Topics studied include a) misconception that at equilibrium concentration of reactants and products at equilibrium are equal, b) misconception that reaction provides in only one way, c) misconception that hen equilibrium is re-established following an increase in temperature, the concentration of NOCl will be greater than at the initial equilibrium d) misconception that when the system at equilibrium is disturbed by increasing the concentration of NO, the reverse reaction rate will instantaneously decrease e) misconception that when the system at equilibrium is disturbed by decreasing the volume, the reverse reaction rate will instantaneously decrease and f) When a catalyst is added to the system at equilibrium, the concentrations of NO, Cl<sub>2</sub> and NOCl (i.e. all the species in the reaction) will change (increase or decrease) depending on the effect of the catalyst. It would be hard to speculate what could have been the reason for such an outcome. The authors themselves did not suggest what changes would be considered in the future study or what effects in the study could have contributed to such an outcome. While misconceptions such as rate vs extent or effect of catalyst are often reported as misconceptions associated with chemical equilibrium, the concepts themselves are purely kinetics in nature. The study did not aim to understand if students have difficulties with foundational chemistry concepts such as gas laws, kinetic molecular theory, stoichiometry and a moderately advance topic such as kinetics. However, this study opened up doors for integrating technology through visualizations to teach chemical equilibrium.

Russell et al (1994) working on a National Science Foundation (NSF) funded research developed a prototype called 4M CHEM. While not explicitly stated, the study is based on a theoretical framework developed by Mayer and Sims (1994). Mayer's cognitive theory of multimedia learning assumes that students learn better when words and pictures are presented simultaneously than when one of them is presented alone. As it was a prototype, the software itself was not studied in real world setting with students. Search to locate this software yielded no luck. The program screen was split in to four quadrants each offering a different visual element. Also whether the software capture all aspects of chemical equilibrium is not clear. The screen capture provided in the article only addressed the aspect of temperature. The program screen also contained buttons such as stop and pause. Students have the option to choose between audio, video or graphics. The video option would provide students with an actual experiment, the graphic option would provide students with a microscopic view of the reaction and audio option would provide students with a narrative of what's happening. It is not clear whether audio would be provided to support the video or graphics or both. While the study was never implemented in a real world classroom, till date it remains a unique kind towards use of computer visualization to teach chemical equilibrium.

Trey et al (2008) examined the effect of a computer simulation incorporating analogies. The study contained two groups, control and experimental. The control group received instruction on chemical equilibrium through text and pictures, while the experimental group received chemical equilibrium instruction through dynamic simulation containing analogies. The analogy involved the use of a weight balance. The weight balance was chosen as an analogy because the authors felt students could more

easily relate to because of their everyday experience. The study was built on a GEM instructional approach developed by Khan (2007). The GEM instructional approach involves three steps. Step a) generate an initial mental model b) evaluate the initial mental model and c) modify the mental model. The model presented in the study is similar to the model presented above by Russell (1994). The difference is video and audio recordings were taken out and replaced by an assessment. Students were presented with an assessment question, following their interaction with the simulation. Another difference is, microscopic particle movement is not present in the study. Particles were simply added like a weight to either side of the balance. In sharp contrast this study by Trey et al (2008) did contain graphical plot providing concentration change as a function of time. Similar to the above two studies, this study is also a unique kind on its own. The authors concluded, computer based analogies provided significant learning gains towards learning chemical equilibrium than narrative text and static pictures of the same analogy. Another commonality between this study and the two other studies mentioned above is the software is nowhere to be found. I examined the website provided by the authors which was affiliated to the University of British Columbia, Vancouver. The website is no longer active and no further details can be obtained about the software. It was also not very clear from the article what specific concepts of chemical equilibrium were tested and whether or not such tested concepts would have provided students with adequate conceptual understanding to answer 10 item test questions offered after the simulation phase.

In another study Akaygun (2009) as part of a doctoral work studied the effect of computer visualizations on students' mental models of dynamic physical equilibrium. It

must be pointed out here, physical equilibrium is different from chemical equilibrium, in that there will no change in the chemical composition, rather changes only happen at the physical states, such as change from gas to liquid or vice versa. For the study PhET simulations developed at the University of Colorado, Boulder was used. Students who participated in the solubility equilibrium study were different from students who participated in the liquid vapor equilibrium study. Mental models of students from both student groups were compared to mental models of experts. While students in both groups showed gains in their understanding at the macroscopic level, there was not a significant change at the microscopic level. Similarly when students in group were asked to answer an open ended conceptual questionnaire prepared for the other group, students were applied principles incorrectly in to the new situation. For instance students in the solid/liquid equilibrium study when asked to complete an open ended conceptual questionnaire on liquid/vapor equilibrium, a portion of the students mentioned molecules splitting when the liquid evaporates. This implies students have incorrectly applied their understanding of solid forming ions in liquid, where a solid splits in to positive and negative ions. Similarly when conceptual pre and post test scores on solubility equilibrium is compared it showed no change.

# **Conceptual Change and Chemical Equilibrium**

While there are plenty of studies that have focused on students' alternative conceptions about chemistry, very few studies have addressed the role of conceptual change in the context of chemical equilibrium. Atasoy (2009) examined the effect of conceptual change approach on understanding of students' chemical equilibrium concepts. The major objective was to compare conceptual change based instruction with traditional instruction. Conceptual change text developed for this study was based on Posner et al (1982) model of conceptual change. The key idea behind conceptual change text is to initiate cognitive conflict and help students to make connections during the conceptual change process. The course material used in the study was developed after examining the literature about conceptual change texts, concept maps, analogies and predict-observe-explain (POE) strategies. The POE strategy was considered because of its role in determining students' prior knowledge. The authors found conceptual change text to be effective based on four reasons a) POE strategies were used to address condition 1 suggested by Posner et al (1982) which is learners must be dissatisfied with their existing knowledge b) analogies made concepts more appealing to students which satisfied Posner et al (1982) condition 2 which is, the new concept must be intelligible, c) concept maps allowed students see the relation among various concepts which satisfied the third condition, learner must the new concept plausible and d) solving problem allowed students to apply the new science concepts to different situations. The authors also suggested that, alternate conceptions were only made explicit to students in the experimental group.

Bilgin et al (2006) examined the effect of cooperative learning approach based on conceptual change condition on students' understanding of chemical equilibrium concepts. Similar to the study reported above, this study also involved experimental and control groups. The study is designed around analogies as the strategy to enable conceptual change. Research studies have shown that analogies provide students with means to develop their own ideas and analogy serving as a reference point to check on

plausibility of their earlier explanations (Brown and Clement, 1989; Harrison and Treagust, 1994). Analogy was used in the study to specifically for the following reasons a) concept acquisition, b) increased student attention, c) intelligibility and plausibility. The use of analogy does offer simplicity to the instructional approach, yet it does come with some disadvantages while explaining dynamic chemical equilibrium concepts. It is important for the teacher to know limitations or major difficulties of the analogy prior to using it. Improper use of an analogy can lead to confusion or to the alternative conceptions.

Canpolat et al (2006), proposed a study which examined conceptual change approach towards teaching chemical equilibrium. The study is an extension of an earlier study conducted by Russell (1988) with a minor change. The change being volume of the measuring cylinder was changed in the current study in contrast to the earlier study by Russell (1988). Russell (1988) proposed three models that could be used when teaching chemical equilibrium. Chiu et al (2002) examined the role of constructing mental models while teaching chemical equilibrium. This study is based on Chi's theory of conceptual change model involving ontological shifts. According to Chi's conceptual change model, a concept such as chemical equilibrium contains constraint based features like randomness, simultaneous, uniform activities. A constraint based interaction provides no information about its time course, because it has no time course.

The concept of electric current is an example of the constraint based interactions category. Electric current is produced when charged particles travel through a field. Hence an electric current is neither a matter nor properties of the matter, but a process

that is fundamentally constraint-based and has no casual agents. Concepts such as light, heat and force also belong in the constraint-based interaction category.

The constraint based features might prevent students from deeply understanding the concept of chemical equilibrium. The study explored students' mental models towards chemical equilibrium in the cognitive apprenticeship context.

Ozmen (2007) examined the role of conceptual change texts in remediating high school students' alternative conceptions concerning chemical equilibrium. Students were put in to control and experimental groups. Both groups were administered the alternative conceptions about chemical equilibrium (ACCET) test before and after. Students in the experimental group received conceptual change text instruction and students in the control group received traditional instruction. The texts used in this study were constructed by a group of chemistry student teachers under the researcher's supervision. Five conceptual change texts were prepared by taking into account students' alternative conceptions determined with the ACCET literature. In the text, such questions were presented to students at the top of the texts. The purpose of this question was to activate students' alternative conceptions. In each of the texts, the topics were introduced by such questions and students' possible answers that are not scientifically accepted were mentioned directly. In this way, students are expected to be dissatisfied with their present conceptions. The conceptual areas covered by the conceptual change texts were; the approach to equilibrium, the application of Le Chatelier's principle, the constancy of the equilibrium constant and heterogeneous equilibrium. Each text aims to remediate the alternative conceptions identified previously and which were related to these conceptual areas. In each of the texts, students were introduced to questions and their possible

answers that may include alternative conceptions held by the students. Following the prediction phase, the students were presented with common alternative conceptions along with evidence countering these alternative conceptions and then discussed in the texts. Students were expected to be dissatisfied with their current conception. Finally, the students were informed of the correct scientific explanations supported by examples. Authors of the study suggested, conceptual change text can be combined with other instructional strategies such as animations, simulations, static visuals, analogies to enhance student understanding towards chemical equilibrium concepts.

Chiu et al. (2002) explored students' mental models of chemical equilibrium after experiencing instruction through a cognitive apprentice (CA) model, proposed by Collins, Brown and Newman (1989). The main features of the CA model include coaching, modeling, scaffolding, articulation, reflection, and exploration. Further information about the CA model can be obtained from Collins, Brown and Newman (1989).

The study explored the foundational chemical equilibrium concepts of a) closed system versus an open system, b) microscopic characteristics, c) reversible reaction, d) existence of all substances and e) Le Chatelier's principle (LCP) for homogeneous and heterogeneous system. A homogeneous system is where reactants and products exist in a single phase (i.e., they exist in solid, liquid, gas or aqueous phase), whereas in a heterogeneous system, reactants and products can exist in more than one phase (i.e., a reactant could be in homogeneous phase, whereas another reactant could be in liquid phase and products could be gas phase).

Conceptual change was categorized by an addition or deletion of a concept from an ontological tree. In a basic conceptual change participants omitted the idea that

systems attaining chemical equilibrium are closed and dynamic versus open and static, then they have exhibited a basic conceptual change. However, if a concept's meaning has been completely removed and replaced by a new concept that is ontologically incomparable to the existing meaning, then the participant was considered to have exhibited a radical conceptual change. Students exhibited conceptual difficulty over chemistry concepts because they have difficulty changing from an event ontological category to a constraint based interactions category.

Thirty 10<sup>th</sup> grade students participated in the study: 10 in a control group and 20 in an experimental group. Both groups were presented with a series of hands on chemical experiments. Students in the experimental group were instructed based on the CA model. Students in the control group received instruction from a tutor without the CA support. The results from the study revealed that the CA group significantly outperformed the non-CA group. Students in the experimental group were capable of constructing mental models of chemical equilibrium including dynamic, random activities of molecules and interactions between molecules, whereas students in the control group failed to construct similar mental models of chemical equilibrium

# **Conceptual Change Theories**

Investigating and addressing student misconceptions is a complex phenomenon. Understanding how students' learn is not a new issue and it's an ongoing one. Over decades, several theories have been put forwards towards how students' learn. Plethora of theories have been put forth by researchers to understand conceptual change, ranging from theories of cognition to theories of socialization (see, e.g., Schnotz 1998, Schnotz et al. 1999, Stark 2002). This suggests that there is not a single definition of what contributes "conceptual change.

Researchers differ in their view of conceptual change. We will look in to the various perspectives on conceptual change in science.

### Vosniadou's Conceptual Change Model

According to Vosniadou and Brewer (1987), for a student to demonstrate conceptual change, the learning process must result in significant reorganization of the knowledge structures rather than enrichment. The question then arises, how a classroom teacher goes about reorganizing the knowledge structures of a student? It also raises another question, what is learning? Learning is an effortful and mindful process and students should be encouraged to construct their own knowledge and skills through active processing, rather than being passive listeners (Vosniadou, 2001). This can be done by asking students to participate in projects, to solve complex problems, to design and execute experiments, to think about their ideas, to listen to the ideas of others, and in general to assume control of their learning (Vosniadou, 2001).

Vosniadou (2001) proposed a list of steps that should be followed while designing learning environments that promote conceptual change. The steps are a) reinterpretation of deeply entrenched presuppositions and beliefs – for example children's view of earth as a flat rectangle, a disc or as a hollow sphere, with people living on flat group deep inside it, suggests children's interpretation of scientific information are often constrained by deeply entrenched presuppositions, b) metaconceptual awareness – students are often not aware of the presuppositions and beliefs that constraint their learning. In other words

conceptual change not only involves change in specific beliefs and presuppositions, but also development of metaconceptual awareness, i.e., making students aware of the beliefs and presuppositions that constrain their learning (Vosniadou, 2001) c) importance of mental representations – in addition to entrenched presuppositions, the mental representations students develop or possess to understand new information influence the knowledge acquisition process (Vosniadou, 2001). The mental model students develop during cognitive functioning can constrain their knowledge acquisition process (Vosniadou, 2001). For example students who hold an incorrect view (flat disc or hollow sphere) about earth will explain day and night cycle by saying the sun goes down behind the mountains (Vosniadou, 2001) d) sequence of acquisition of the concepts that comprise a given subject matter area – for example it is not possible for students to understand the spherical nature of earth, if they do not have a concrete elementary knowledge about gravity e) taking in consideration of students' prior knowledge f) cognitive conflict – teachers must have an informed knowledge about how students see the physical world and learn to take their viewpoints in to consideration while designing instruction g) providing external models and representations – models and external representations can be used to clarify aspects of a scientific explanation that are not apparent when the explanation is provided in a linguistic or mathematical approach. While the steps suggested above were intended for a teacher while designing learning environments, it captures the essence of what a conceptual change process should look like.

While there are a variety conceptual change frameworks, majority of them have their foundation in constructivism. The constructivist view of learning assumes that each

individual constructs his or her knowledge actively from his or her own experiences. This process is based on and constrained by the already existing knowledge (Widodo & Duit 2004).

Siebert (2003) and Treagust et al (2000) suggested learning does not involve passive intake of knowledge rather actively constructing it. In other words, a student is one of who is responsible for his or her learning process. Teachers can only support the learning process when learning takes place on the basis of prior knowledge. Teachers need to be informed about how students see the physical world and learn to take their points of view into consideration when they design instruction. Instructional interventions need to be designed to make students aware of their implicit representations, as well as of the beliefs and presuppositions that constrain them. It is important to provide meaningful experiences that lead students to understand the limitations of their explanations and to motivate to change them.

Finally, it is necessary to provide cultural support for the reorganization of existing knowledge, necessary for learning science (Vosniadou, 2001). Once students' prior knowledge is addressed, the next step would be to address students' entrenched presuppositions. The new information presented should be consistent with prior knowledge and not contrary to prior knowledge. When the new information is consistent with prior knowledge, it can be incorporated easily into existing conceptual structures. This type of information is most likely to be understood even if it is presented as a fact without any further explication. However, when the new information runs contrary to existing conceptual structures, simply presenting the new information as a fact may not be adequate. Students can take two course of action if the information presented is

contrary to existing information a) simply add the new information to existing knowledge structure and the new information will remain inconsistent with the old information and b) or distort the new information so it is consistent with the new information. The latter situation is much worse because it only increases the complexity of an existing misconception Vosniadou (2001).

### Posner et al's Conceptual Change Model

Posner et al. (1982) embedded their explanation of conceptual change within a conceptual ecology perspective. According to Posner et al (1982) a learner's conceptual ecology consists of their conceptions and ideas rooted in their epistemological beliefs. The first step towards conceptual change in a conceptual ecology perspective is the learner must be dissatisfied with an initial conception in order to abandon it and accept a scientific conception for successful conceptual change. In addition the scientific conception must also be intelligible, plausible, and fruitful for successful conceptual change to occur. Intelligible means that the new conception must be clear enough to make sense to the learner. Plausible means the new conception must be seen as plausibly true. Fruitful means the new conception must appear potentially productive to the learner for solving current problems. Posner et al (1982) perspective assumes that these cognitive conditions should be met during the learning process for a successful conceptual change. From a conceptual ecology perspective, the constituent ideas, ontological categories, and epistemological beliefs highly influence a learner's interactions with new ideas and problems.

### **DiSessa's P-Prims Model**

According to DiSessa (1993), knowledge structure of novices consists primarily of unstructured collections of many simple elements known as phenomenological primitives or p-prims. The learner assumes that "something happens because that's the way things are" (DiSessa 1993, p. 112). According to DiSessa (1993), p-prims do not have the status of a theory because they are neither produced nor activated under a highly organized system like the classical framework proposed by knowledge as theory researchers. Like many knowledge as theory views, diSessa's view knowledge is acquired by students because of everyday experience. DiSessa et al. (1998, 2002) argue that knowledge cannot be described appropriately by only one type of mental entity as the supposed concepts. What is usually understood as a scientific concept should rather be regarded as a complex system consisting of a large number of interacting elements. From their perspective, conceptual change means modification, reorganization and recombination of different mental entities in complex ways. Derived from studies within the field of physics two kinds of mental entities are suggested p-prims (phenomenological primitives) and coordination classes. P-prims stand for small, simple knowledge elements. For example, students when asked the reason why it's hotter in the summer than in the winter (Sadler, Schneps, & Woll, 1989). Many of the students responded that it is because the earth is closer to the sun. When students were requested to expand upon their reasoning, they suggested earth moving closer to the sun, is similar to moving close to a stove you felt the heat more than when you move away from the stove. Novices are assumed to have numerous such isolated p-prims deduced from everyday experience.

In comparison, experts or scientists, are presumed to differ from novices in that they have integrated p-prims into comprehensive knowledge structures. P-prims change their function from primitive explanatory elements into parts of a complex system which is more appropriate to provide elaborated explanations. P-prims are generated from a learner's experiences, observations and abstractions of phenomena. Several p-prims are connected to form a larger knowledge network. DiSessa (1993) describes cuing priority, reliability priority and structured priority to propose how such p-prims are recognized and activated according to context. In other words an identical p-prim activated under one context may not be activated under another context.

### **Conceptual Frameworks Used in the Current Study**

A combination of conceptual frameworks was used to guide the current study. The first being Chi's (1994) ontological shift model and the second being Hammer and Brown's (2008) complex systems theory.

# Chi's Ontological Shift towards Conceptual Change

Conceptual change does not occur during all types of learning, but only when prior knowledge contradicts with new scientific knowledge. In a classroom situation, students may not have prior knowledge about the concept they are learning (Chi, 2008). Under such circumstances, learning involves adding new knowledge. If in fact students have prior knowledge about the concept to be learned, but if that knowledge is incomplete, then learning can be conceived as gap filling. Conceptual change does not occur during knowledge acquisition when there is no existing prior knowledge or during gap filling.

The third knowledge acquisition condition involves a situation where a student may have acquired ideas from prior instruction or everyday experience that are in direct conflict with scientifically established ideas. In contrast to gap filling or adding new knowledge, under the third circumstance prior misconceived knowledge must be changed to scientifically accepted knowledge to promote understanding. This third condition refers to conceptual change.

## Conceptual Change at the Level of Belief and Mental Model

The level within the ontological model can categorize the level of conceptual change from that of a single idea, or at the broader level of the mental model. Students' prior knowledge can be represented at the grain size of a single idea or belief (Chi, 2008) If false beliefs and scientifically acceptable information co-exist in a contradictory fashion, then instruction designed to target false beliefs might succeed in replacing them with more scientifically accepted norms (Broughton, Sinatra & Reynolds, 2007; Guzetti, Snyder, Glass & Gamas, 1993). Chi noted that belief revision can only be successful when misconceived knowledge is in conflict with scientific knowledge.

In contrast to belief revision, where the grain size consisted of a single idea, an organized collection of beliefs is considered a mental model. A mental model is an internal representation of a concept or an inter-related system of concepts that corresponds to an external structure it represents. Similar to belief revision, a mental

model must be in conflict with scientifically acceptable model to enable conceptual change (Chi, 2008; Genter & Stevens, 1983). Instruction that might have an effect and promotes conflict at the mental model level, if conflict is not generated at the belief level, new information is infused or assimilated into an existing flawed model Chi (2000 & 2008). Hence mental model revision can only be successful when the learner perceives contradiction at the belief and mental model levels.

Similar to belief and mental model revision, conceptual change requires a shift across lateral or ontological categories. Conceptual change requires a shift across lateral or ontological categories. As noted earlier, while matter, process and mental states serve as ontological categories, branched sub-categories under each ontological category are referred to as lateral categories. If two lateral categories occur at the same level with in an ontological tree are considered to be parallel (Chi. 2000).

#### Assumptions of Conceptual Change

Conceptual change is difficult because it requires learners to recognize their conceptual misunderstanding, and the need to reassign an idea to a new ontological category, or to create a new ontological category they currently lack (Chi, 1994). The theory contains three assumptions. The first assumption is epistemological in nature; dividing knowledge into three categories: a) matter, b) processes and c) mental states. The category of matters pertains to whether an object under question is classified as artifacts or natural kinds. In comparison, processes can be categorized as events, procedures and constraint based interactions. Mental states can be categorized as

intentional or emotional. Conceptual change occurs when a concept is reassigned from one ontological category to another.

The second assumption is metaphysical in nature, that is, many scientific concepts belong to the ontological category known as constrain-based interactions; a subcategory of processes. Constraint-based interactions are determined by a known or knowable set of constraints (Chi et al., 1994), but do not consider time as an element.

The concept of electric current is an example of a constraint-based interaction category. Electric current is produced when charged particles travel through a field. Hence an electric current is neither considered as a matter nor as properties of the matter. It is considered as a process that is fundamentally constraint-based and has no casual agents. Concepts such as light, heat, and force also belong in the constraint-based interaction category.

The third conceptual change assumption is related to students' naïve conception that they incorrectly assign many scientific concepts to the category of matter. If students become aware of their ontological commitments, they can then become aware of how the scientific theory does not fit with their existing knowledge structure. They would then be able to assign the concept into a correct category by revising their ontological commitments, categories and presuppositions.

Researchers supporting Chi's perspective propose that conceptual change is a gradual and time consuming process because the student must revise and restructure an entire network of beliefs and presuppositions. While Chi's argument focuses specifically on changing ontological categories, Vosniadou and Ioannides (1998) present a

contrasting view of conceptual change, suggesting that ontological change is only one of the changes required in the process of changing theories.

In later work, Chi (2008) added two additional kinds of lateral categories within the process tree: direct and emergent. Direct and emergent processes are mutually exclusive. Direct processes usually involve an identifiable agent that causes an outcome in a sequential and dependent fashion. In contrast, in emergent processes have neither an identifiable agent(s) nor a specific sequence or stages. In an emergent process, all agents have equal status and simultaneously interact to produce a collective outcome.

# **Complex system theory**

Complex system theory (Brown & hammer, 2008) will be considered as the other theoretical framework guiding the use of simulation towards conceptual change. Complex systems theory deals with complex dynamical systems, in which there are interaction among components of that system, i.e., what happens to one part of the system can affect another part of the system, which in turn can affect the initial part of the system where the change was induced. Another reason why the complex System theory by Brown and Hammer (2008) is considered is because of the fact, while students hold alternate or misconceptions towards chemical equilibrium, they also hold an algorithmic view of the system. Research studies that were addressed in earlier sections clearly pointed out that students approach chemical equilibrium which is a complex system from a mathematical perspective or use a pre-determine algorithm which fits well with in the existing knowledge structure. For instance, students who tend to use Le Chatelier's principle (LCP) as a rule to determine equilibrium shift when volume of the system is

reduced, tend to conclude the system will shift to the side with least number of moles. Students who viewed a complex system from an algorithmic perspective, failed to consider the fact that a system is made of multiple components and making a change to one component of the system affect other components contained the system. In other words to develop concrete conceptual understanding of chemical equilibrium concepts through simulations, a system's approach is required.

The four components that make up core of the complex systems are a) intrinsic dynamism, b) non-linearity, c) emergent structures and d) embeddedness. Intrinsic dynamism: According to intrinsic dynamism, elements of a system are in constant and dynamic interaction. Systems in dynamic equilibrium are "thing like" in that in many aspects they remain the same, but the mechanisms that produce them are not "thing alike", in that they are dynamic. As with a system that attains chemical equilibrium, the system may appear macroscopically static or not dynamic, but at the microscopic or molecular level, the system is dynamic and continue to stay dynamic, in that the forward and reverse reactions continue to occur, reactants formed continue to make products and vice versa. As David and Brown (2008) point out that in many cases, it is appropriate to ignore the dynamic aspect of the system and treat the system as having an enduring identity. However if the goal is toward changing the system, as in conceptual change, treating a system as unitary is not appropriate. All simulations presented in the study except for one, were developed to demonstrate the intrinsic dynamism seen in a chemical reaction exhibiting equilibrium. Except simulation 5, all simulations will present the chemical reaction in the particle mode, so students can witness how reactions continue to occur even after a system as attained equilibrium and does not remain static.

The common alternate students hold is a single direction belief, i.e., reaction commences continue to occur in one direction and stop occurring once a certain level of products have been produced. The simulations will demonstrate the foundational idea of chemical equilibrium, i.e., when a system attains equilibrium, the concentration of reactants and products do not change and rate of forward and reverse reactions remain equal and constant.

Non-linearity: In contrast to systems which are linear, such that disturbing the system lead to proportional results. For example doubling the tension on a rope in a pulley system, will also double the tension on the rope. Whereas, in a non-linear system, a perturbation leads to non-proportional results. In contrast to algorithmic approach used by students to solve chemical equilibrium problems (Pushkin, 1998) were linearity is assumed, disturbing a component of a system that has attained equilibrium, does not follow a linear behavior. In other words increasing the concentration of a reactant in a system that has attained equilibrium, does not increase the concentration of all species by an equal amount. The simulations were designed to exhibit the property of non-linearity. Emergence: Since elements of the system are in constant and dynamic interaction, structures and patterns emerge. The structures emerging cannot be predicted based on the individual elements and so the structures must be studied at appropriate grain size. Embeddedness: Complex systems are composed of several smaller systems that are also complex in nature. A complex system such as chemical equilibrium involves a network of concepts such as stoichiometry, gas laws, molar concentration, kinetics, thermodynamics, catalysis etc. While the simulations were not developed to address each of the networking concepts, networking concepts were infused in to each simulation. In

account of time constraints, the current study did not address networking concepts involving thermodynamics and catalysis.

# Organization of the remaining chapters in the study

Chapter 2 provided a literature review on the tripartite model of matter, conceptual change approach towards chemical equilibrium, visualization and conceptual understanding, theoretical and multimedia framework used in the current study. Chapter 3 provides information about the research methodology, study design, quantitative instrument and the nature of data analysis. Chapter 4 provides analysis of results and analysis of quantitative and qualitative data from the dissertation study. Chapter 5 summarizes the findings from the research study along with implication and recommendations for future research.

### **CHAPTER III. METHODOLOGY**

### **Purpose of the Study**

Research on student misconception on chemical equilibrium has been underway for more than three decades. As noted earlier in the introduction and literature review sections many such studies focusing on understanding student misconceptions were quantitative in nature rather than qualitative in nature. Qualitative and mixed methods studies have the added potential for rich depositions to characterize student conceptual difficulties and possibly identify stumbling blocks in student thinking. Moreover, many of the previous studies have tended to employ quantitative instruments using single-tier (Hackling & Garnett (1985), Treagust (1988), Banerjee (1991), Hameed et al (1993), and Chueng (2009)) and two-tier Ozmen (2008) for data collection.

The purpose of the dissertation study was to answer the research questions put forward and be able to establish statistical significance that the simulations aided towards conceptual gain among students in the experimental group. Because currently there are no simulations available on the World Wide Web or from other sources that satisfy the requirements of the study, simulations were developed by the researcher. Simulations were developed using SCRATCH software. SCRATCH is a java based software program developed at the Massachusetts Institute of Technology (MIT). Version 2.0 of the software was used towards simulation development. The concepts chose to be addressed by the current study are a) approaching equilibrium, b) characteristics of equilibrium, c) effect of concentration change on equilibrium and d) effect of volume change on equilibrium. A total of 11 simulations were used to address the above four concepts. The

dissertation study and the pilot phase of the study utilized a mixed-methods approach towards data collection. A component of the dissertation study was the pilot phase. The purpose of the pilot phase was to obtain feedback from students regarding the simulations and the quantitative instrument. In addition the pilot phase also provided evidence of increased student conceptual understanding of chemical equilibrium concepts.

#### **Mixed Methods Design**

The study utilizes a mixed-methods approach to data collection. According to the fundamental principle of mixed methods research design, a researcher should use a combination of methods (qualitative and quantitative) that have complementary strengths and weakness. The core assumption behind mixed methods research is when a research combines statistical methods (quantitative data) with narratives and personal experiences of a participant; the cumulative strength provides a better understanding of the research problem than data from either form of data alone (Creswell, 2015). The intent is to merge the results of both methods for analysis. In an explanatory sequential design, data collection commences with the quantitative strand and then data is collected from the qualitative strand to explain the results from the quantitative strand. The purpose of the exploratory sequential design is to explore a problem through qualitative data collection and analysis (Creswell, 2015). An explanatory sequential design was chosen for the current study primarily because prior misconception research has quantified student misconception towards chemical equilibrium. Quantitative results yield statistical significance, confidence intervals, and effect sizes and provide the general outcomes of a study. However, quantitative results alone won't be sufficient to know how the findings

occurred. Hence, the next logical step in the sequence would be to collect qualitative data that would explain the findings from the quantitative strand.

The explanatory sequential design used during the study is an alternate version of the explanatory sequential intervention based design presented in Creswell (2015, p62). The explanatory sequential intervention design presented in Creswell (2015, p62), the consisted of a quantitative phase followed by the qualitative phase. In contrast, the design used in the study, the qualitative interviews occurred following the pre and post quantitative phase.

Figure 1 and 2 presents the explanatory sequential design used with the experimental and control group respectively during the dissertation study. Number of participants who participated during each of the phase is shown in parenthesis. The procedure used towards data collection is identical to the procedure described in the previous paragraph. The only difference being, participants in the experimental group received intervention through simulations while participants in the control group were allowed to use their lecture notes (active control) on the topic of chemical equilibrium.

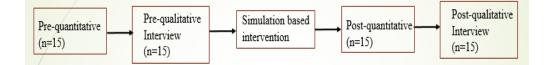


Figure 1: *Explanatory sequential intervention based design used with the experimental group during the dissertation study.* 



Figure 2: *Explanatory sequential intervention based design used with the control group during the dissertation study.* 

During the pre-quantitative phase, participants completed the chemical equilibrium misconceptions test (CEMT). More information about CEMT can be found under the instrument section of the research design. Number of participants who participated during each of the phase is shown in parenthesis. Following the prequantitative phase, one-on-one interviews were conducted with each of the participant. Participants in the control group were allowed to use their lecture notes, while participants in the experimental group received intervention through computer simulations. More about the sequence of simulations can be found under sequence of activities section of the research design. Following intervention and a brief recess, participants completed the post-quantitative phase by re-taking CEMT. Participants then completed the post-qualitative interview phase by completing a one-on-one interview with the researcher.

Further information about participant recruitment, chemical equilibrium simulations developed for the study, sequence of simulation activities, study instrument, interview protocol can be found under the research design section in the current chapter.

# **Research Questions**

The objective of the study is to investigate the following research questions

- a) What are students' conceptual understandings of chemical equilibrium before interacting with the simulations?
- b) What key characteristics of students' mental model regarding chemical equilibrium concepts can be extracted from student writings, drawings and oral explanation before and after viewing simulations?
- c) What evidence is observed to suggest changes in students' mental models on chemical equilibrium after they use the chemical equilibrium simulations?
- d) What are students' conceptions of chemical equilibrium after interacting with the simulations?

#### **Research Hypotheses**

The research hypotheses used quantitative and qualitative methodologies.

**Hypothesis 1:** Hypotheses tested through the quantitative methodology that mean difference in post-test will occur between the control and experimental group, after adjusting for the pre-test scores among both groups (control and experimental) on the CEMT.

During the pilot phase of the dissertation study, a paired samples t-test was used to determine statistical significance. The reason a paired samples t-test was used, because the pilot phase employed a single group pre post-test design. In the dissertation study, analysis of covariance (ANCOVA) was conducted to determine whether the post-test means differed between the two groups (experimental and control) on the CEMT after adjusting for the pre-test scores.

**Hypothesis 2:** Hypotheses tested through the qualitative methodology is there is a change in thought process or mental model among participants in the experimental group.

A mental model is an internal representation of a concept or an inter-related system of concepts that corresponds to an external structure it represents, (Chi, 2008). Hence, the initial mental models that students bring to a learning environment are different from each other and therefore, different learns construct identical meanings differently (Bodner, 1986). A semi-structured interview was conducted among both groups after the pre and post-test. Transcribed data was coded to establish themes. Thematic analysis is a search for themes that emerge as being important to the description of a phenomenon (Daly, Kellehear,, & Gliksman, 1997). The phenomenon explored in the current study was conceptual understanding. Themes generated from the qualitative data would enable the researcher to determine if there is a difference in participant's mental model before and after the intervention.

## **Research Design**

# **Participants**

The pilot phase of the dissertation study began during the earlier part of March 2016. The purpose of the pilot phase was to receive feedback from participants on the instrument and computer simulations. The feedback received was used to improve the instrument and computer simulations before implemented during the dissertation study.

Participants in the pilot phase were enrolled in one of the four sections of the second semester general chemistry course at the University of Kentucky. As the course work met the pre-requisite, students with wide variety of majors were enrolled in the class. The class chosen had an enrollment of about 400 students. After obtaining consent from the course instructor, the researcher met participants during class time and presented information about the scope of the study. In addition, participants were briefed about the institutional review board (IRB) protocol. Approved IRB protocol can be found in Appendix G.

The researcher left a sign-up sheet with the instructor. Participants who expressed interest in participating in the study provided their name and email address on the sign-up sheet. A smaller fraction of students who had additional questions about participating in the study, met with the researcher on a one-on-one basis before committing themselves to the study. Over a period of two weeks 15 students have signed up (some through the signup sheet and some through email communication). Once all 15 students confirmed their agreement to participate have signed up, a common schedule was worked up so they can participate in the study. Students met over two days to complete the study. On Day

1, participants completed the pre-test and pre-qualitative interviews. The average time took by a student to complete the pre-test was around 10 minutes. The pre-qualitative interview lasted between 10-15 minutes per person. The average time took by a student to complete the post-test was around 10 minutes. The post-qualitative interview lasted between 10-15 minutes.

The dissertation study took place around the end of April 2016 and beginning of May 2016. Similar to the pilot phase, participants in the dissertation study where recruited from the remaining three sections of the second semester general chemistry course. The three sections combined had a student population of approximately 1200. The researcher left a sign-up sheet with the instructor. Participants who expressed interest in participating in the study provided their name and email address on the sign-up sheet. At the end of the two week period, a total of 30 students have signed up for the study. The thirty students were then randomly assigned to the control and experimental group. After surveying each student about their availability, two common schedules were chosen; one for the experimental and the other for the control group.

### Intervention

Intervention was provided to participants in the form of computer simulations. Participation with the intervention on an average lasted about 90 minutes during the pilot phase and about 60 minute during the dissertation study. The reduction in intervention time was primarily due to improvements made to the simulations from data collected from students in the pilot phase. The timeline during which the pilot study and the dissertation study took place is an important factor. During the pilot phase, participants

were learning the concept of chemical equilibrium in the chemistry lecture courses, whereas when the dissertation study took place, participants have already completed a midterm that included questions on the topic of equilibrium. In fact, around the time when the dissertation study took place, the final examination week was approaching.

# **Sequence of Activities**

In addition to establishing a reliable instrument and a clear working simulation, an additional objective behind the pilot phase was to establish an average time frame. The time frame suggested to participants in the pilot phase was a total of three hours. This included the pre and post testing, pre and post qualitative interview session and the intervention session. To avoid physical and mental exhaustion, two common sessions were chosen.

During the first session, participants in the study were given the pre-test. Participants required approximately 8-12 minutes to complete the pre-test. As students completed their pre-test, they sat with me one-on-one for the pre-qualitative interview. I had reserved a space in the corner of the computer lab were the interview took place. Each student had to wait their turn to complete the interview. The average interview time lasted around 10-15 minutes.

When students met during the second session, they completed the intervention followed by a 30 minute break between the intervention and the post quantitative and qualitative assessment. The intervention lasted approximately 90-110 minutes. On an

average, the post quantitative and qualitative assessment collectively lasted about 15-25 minutes

Student feedback on the instrument and simulations from the pilot study were taken in to account to make necessary corrections.

Notable corrections include,

- a) Changing the color of the buttons used in the study. In the pilot study, the buttons had a red background with a black font. Handful of students suggested having a flashy font color would make it easier to view the buttons. The correction was made on the version used in the dissertation study. The newer buttons had a red background and yellow font
- b) Many students suggested to adding a caption on the screen that told what button to press to move further in the simulation. For instance, the following caption was added to simulations. Press tab on your keyboard to continue.
- c) The common complaint students had during the pilot study was, they do not want to hear the introduction speech about the architecture of the simulation, when they had to re-do a particular simulation or when they go from one simulation to the other. Hence, the skip intro option was introduced in to all simulations except for simulation 1. The primary reason being simulation 1 explains why there is a compartmentalized view, when a system attains equilibrium, what characteristics can be seen in a system that attains equilibrium. However, if students want to hear about the architecture of the simulation when they re-do, they can make use of the intro button option.

- d) All 11 simulations requested students to write down qualitatively what they observed and learned through a simulation in the simulation notes sheet. They cannot do it once they finish all 11 simulations. There was a brief pause in the simulation, during which they can write down their observations. Many students suggested they need more time to write down their observations. The version used in the dissertation study provided participants with ample time to write down their observations.
- e) Some students suggested, there was a minor lag between the visual on the screen and the audio recording. The lag issue was fixed in the simulations used in the dissertation study.
- f) While not everyone, fewer students suggested to add brighter colors to molecules shown inside the pistons. Particles were shown in brighter colors in the version used in the dissertation study.
- g) Audio was re-corded for all simulations reflecting changes recommended by students during the pilot study.

The 30 students who volunteered to participate in the dissertation study were randomly assigned to the experimental and control groups. The control group and the experimental group met on different days. As the final examinations week was within two weeks of the date the study was implemented, most students who were willing to participate in the experimental group noted they would not be able to commit to two sessions, as the total average time to participate was around 150 minutes. A common day was scheduled and all participants were notified about the date, time and location. On the day of the intervention, the experimental group volunteers completed the pre-test and qualitative interviews and then sat in front of computers allotted to them. The simulations were pre-loaded to save time.

Modifications made to the simulations based on data collected from the pilot study results in shortening student time on the simulation to 75 minutes from the original average of about 100 minutes. After completing the simulation, participants were asked to shut down the computers and take a 30 minute break. After a 30 minute recess, students took the post-test and the qualitative interviews.

Students in the control group met over two sessions, as the total time invested by them was approximately around 90 minutes. Students in the control group met on a preset day and time and took the pre-test and completed the pre-qualitative interviews. The entire session lasted approximately around 20- 30 minutes per student. When they met the second time, they had the option to review their notes on chemical equilibrium or review the information in the course textbook. All participants except for one decide to use their class notes during the start of the session. They were told, they could start the post-test whenever they were ready. Some students took 10 minutes to review their notes, while others took about 30 minutes. After a self-paced review session, students completed their post-test and interviews.

# **Computer Simulations**

Chemical equilibrium simulations used in the study were developed using the SCRATH<sup>©</sup> software platform developed by Massaschusetts Institute of Technology (MIT), Cambridge, MA. The software platform uses Java based programming language. As pointed out earlier in the literature review section, Schnotz integrated mulitmedia

framework guided the study. In accordance, audio component was seamlessly blended with the visual component in all simulations used in the study. All simulations feature the following essential buttons; a) start, b) stop, c) reset, d) play, e) pause, f) mute. While the mute option is available, students were recommended not to use it. Except for simulation 1 and 5, the other nine simulations featured intro and skip intro buttons. The primary reason being, Simulation 1 presented the visual architecture of a dynamic system attaining equilibrium. Simulation 5 presented an analogy model, comparing a twin body pulley experiment to equilibrium constant K. As the time consumed to complete simulation 5 was less than a minute, skip intro or intro option was not required. All simulations, except simulation 5 were developed around the chemical reaction

 $2NO(g) + Cl_2(g) \rightarrow 2NOCl(g)$  Equation (1)

Simulation 1 presented a macroscopic view of the system attaining chemical equilibrium. Macroscopic level describes phenomena that can be observed through the various senses. For instance, the different phases solid, liquid and gases can be observed through a visual cue or in special cases gases that are colorless can be sensed through smell. In the case of the system considered for the current study, nitric oxide (NO) is a colorless gas and chlorine (Cl<sub>2</sub>) is a yellow colored gas. Hence the product nitrosyl chloride will be a milder yellow colored gas. Participants can witness how the reaction continue to occur in both directions even after the system has attained equilibrium. The lens on and off buttons allowed participants to peek through the macroscopic system in to the particle or microscopic mode. Screen shot of simulation 1 is shown in Figure 3a and 3b. Figure 3a showing macroscopic view of a system attaining equilibrium and Figure 3b showing the purpose of the lens on option.

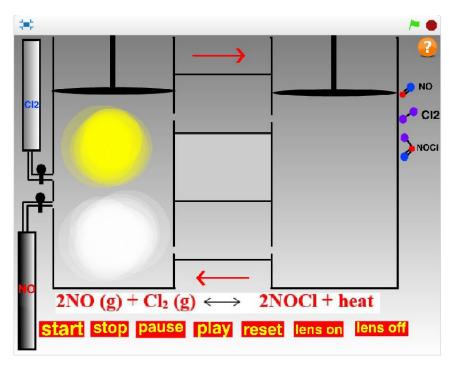


Figure 3(a): Macroscopic view of a chemical equilibrium system at the start

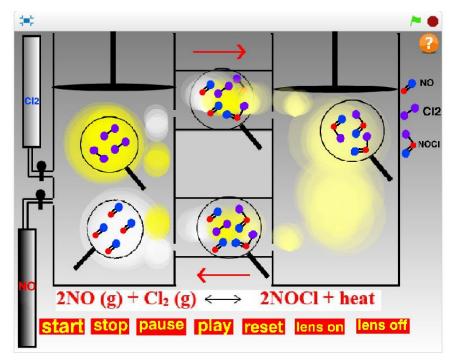


Figure 3(b): Macroscopic view of a system that has attaind equilibrium. The figure also shows the microscopic view of the system using the lens option.

The only difference between simulation 1 and 2 being, the former presented the chemical reaction from a macrosopic view and the latter presented the chemical reaction from a microscopic view. The purpose of simulation 2 is for students to understand that while systems that reach chemical equilibrium may appear macroscopically stable and static, microscopically the system is dynamic not only because of molecular movement but also because the process of bond breakage and creation goes on.

Simulations 3 and 4, in addition to presenting a particle view of a system attaining chemical equilibrium, also provided graphical view of concentration as a function of time and rate of the reaction respectively.

Simulation 5 presented an analogy model. Classic two body pulley experiment on an inclined ramp was used to address the concept of equilibrium constant. In the post interviews participants revealed, of all the simulation they particularly liked simulation 5, as it allowed to easily comprehend the concept of equilibrium constant.

Simulation 6 contained two parts to it. During the initial part of the simulation, a system attaining chemical equilibrium will be shown in the particle mode. During the second part of the simulation, participants can disturb a system at equilibrium by increasing the concentration of nitric oxide (NO) and observe what happens to the system when it re-establishes equilibrium. Simulation 7 and 8 are similar to simulation 6. The only difference being simulation 7 presented changed in concentration as a function of time during both parts of the simulation and simulation 8 presented the change in rate during both parts of the simulation.

Simulation 9 contained two parts to it. During the initial part of the simulation, a system attaining chemical equilibrium will be shown in the particle mode. During the second part of the simulation, participants can disturb a system at equilibrium by decreasing the volume of the system and observe what happens to the system when it reestablishes equilibrium. Simulation 10 and 11 are similar to simulation 9. The only difference being simulation 10 presented changed in concentration as a function of time during both parts of the simulation and simulation 11 presented the change in rate during both parts of the simulation. Table 1 summarizes the sequence of all 11 simulations used in the study. The following table represents the sequence of simulations used in the study

#	Simulation	Notes
1	The concept of chemical equilibrium	Macroscopic version of the system
2	The concept of chemical equilibrium	Microscopic or particle version of the system
3	Concentration and Particle mode	Change in concentration at the particle level with graphical representation of concentration as a function of time
4	Rate and Particle mode	Change in concentration at the particle level with graphical representation of rate of the reaction
5	Two body pulley experiment*	Analogy model, relating the concept of equilibrium and equilibrium constant K
6	Effect of concentration on equilibium of a system	Particle representation of concentration change
7	Effect of concentration on equilibium of a system	Change in concentration at the particle level with graphical representation of concentration as a function of time
8	Effect of concentration on equilibium of a system	Change in concentration at the particle level with graphical representation of rate of the reaction
9	Effect of volume on equilibium of a system	Particle representation of concentration change
10	Effect of volume on equilibium of a system	Change in concentration at the particle level with graphical representation of concentration as a function of time
11	Effect of volume on equilibium of a system	Change in concentration at the particle level with graphical representation of rate of the reaction

 Table 1: Sequence of simulations used in the study (\* was not part of the pilot study)

## **Data Collection**

### **Study Instrument**

An 11 item quantitative instrument, chemical equilibrium misconception test (CEMT) was developed to identify student misconceptions towards chemical equilibrium concepts. The quantitative instrument was developed using misconceptions reported in the literature (Hackling and Garnett, 1985; Hameed et al, 1993).

Student feedback was obtained during the pre and post interview process of the pilot study in order to improve the quality of the instrument. Face validity of the instrument was also established by having experts (chemistry educators) who teach the corresponding general chemistry courses review and make suggestions for modifications of the instrument. Reliability was established by conducting a Kuder-Richardson (KR-20) analysis on the dichotomous pre and post quantiative test results. K-R 20 is a special form of Cronbach's alpha that is used when the quantitative instrument contains dichotomous data (right or wrong responses) and when the response data does not represent a continuous scale or cannot be ranked in any particular order. Revised version of the CEMT used in the dissertation study is shown in Appendix A.

### **Interview Protocol**

Qualitative interviews were conducted with all participants (n=15) in the pilot phase and (n=27) as well as the dissertation phase of the study. A semi-structured interview method was employed. According to Patton (1990), a semi-structured interview is a process in which the tasks and the set of interview questions are predetermined, but the presentation sequence is not established prior to the interview.

The following questions served as the template, on to which additional questions were added as the interview progressed

a) What aspect(s) of the simulation you liked the most?

b) What aspect(s) of the simulation you did not like the most?

c) What aspect(s) about the simulation could be improved?

d) What aspect(s) about the simulation you found the most helpful

e) Are there any particular question(s) you would found confusing on the quantitative instrument in terms of readability and clarity?

f) What was the reason behind your answer choice (repeated for items that were answered incorrectly)

g) On the post-test if there is a change of answer, I questioned them why there is a change of answer choice?

As pointed out under the limitations section in Chapter I, time remained a major constraint throughout the study and hence it was not possible to obtain response for all 11 items from all 15 participants. In such circumstances either the questions were the student has chosen a different choice (correct or incorrect) on the post-test or questions pertaining to the most common misconceptions reported in the literature were chosen.

#### **Data Analysis**

#### **Quantitative Data**

The following statistical analysis were conducted on the data collected from the dissertation study: a) Kuder-Richardson (KR-20) analysis was conducted on the quantitative data pre data (control and experimental) and post (control and experimental) to establish reliability. K-R 20 is a special form of Cronbach's alpha that is used when the quantitative instrument contains dichotomous data (right or wrong responses) and when the response data does not represent a continuous scale or cannot be ranked in any particular order. b) ANCOVA analysis – research hypothesis 1 states, a mean difference in posttest scores will occur between the control and experimental group, after adjusting for the pretest scores. d) conditional probability was performed to determine construct validity, d) frequency analysis on all 11 items (pre and post) to compare percentage common misconceptions, additional misconceptions and correct conceptions between the two groups (control and experimental)

## **Qualitative Data**

A semi-structured interview was conducted among both groups after the pre and post-test. Transcribed data was coded to establish themes. Thematic analysis is a search for themes that emerge as being important to the description of a phenomenon (Daly, Kellehear,, & Gliksman, 1997). The phenomenon explored in the current study was conceptual understanding. Thematic analysis is a method of identifying, analyzing and reporting patterns within qualitative data (Boyatzis, 1998). The pattern is what referred to as theme. Themes or patterns within a qualitative data can be identified in one of two common ways; the first being inductive thematic analysis, also known as, bottom up approach (Frith & Gleeson, 2004) or deductive thematic analysis, also known as top down approach (Boyatzis, 1998). In an inductive approach, the themes identified are strongly linked to the data themselves (Patton, 1990). An inductive approach is largely not driven by the researcher's theoretical interest in the area or topic (Patton, 1990). Inductive analysis is therefore a process of coding the data without trying to fit it into a pre-existing coding frame or the researcher's analytical perceptions (Patton, 1990).

Theoretical thematic analysis would tend to be driven by the researcher's theoretical or analytic interest in the area, hence theoretical thematic analysis is largely researcher driven. Theoretical thematic analysis does not provide a rich analysis of the overall data, but provides detailed analysis of some aspects of the data.

The study reported in the dissertation is not the first in the literature to have explored student misconceptions towards chemical equilibrium, hence a purely inductive approach was not required. Prior research (Canpolat et al, 2006; Hackling & Garnett, 1985; Hameed et al, 1993) on student misconception towards the chemical system described in the instrument have identified larger themes. A theoretical thematic analysis was conducted to code for existing themes identified in the literature. Distractors used in the quantitative instrument served as served as sub-themes and hence coding was purposeful to find words that would justify the sub-themes.

The larger themes identified by prior research (Canpolat et al, 2006; Hackling & Garnett, 1985; Hameed et al, 1993) were retained in the current study and data coded to identify already existing themes. The four larger themes used in the study were a) approaching equilibrium, b) characteristics of equilibrium, c) equilibrium constant and d)

changing equilibrium conditions. The items created on the chemical equilibrium misconception test (CEMT) was consciously created to include previously identified misconceptions as choices. Hence the choices themselves served as sub-themes (theoretical thematic approach). Items that were grouped under each larger theme were,

# Approaching equilibrium

Item 1: As the reaction approaches equilibrium, in terms of rate?

Item 2: As the reaction approaches equilibrium, in terms of concentration?

## **Characteristics of equilibrium**

Item 3: At equilibrium, in terms of concentration?

Item 4: At equilibrium, in terms of rate?

Item 5: <u>At equilibrium</u>, in terms of shift?

# **Equilibrium constant**

Item 6: <u>At equilibrium</u>, in terms of equilibrium constant?

Item 8: After a system at equilibrium is disturbed by increasing the concentration of NO, and when the system re-establishes equilibrium, equilibrium constant K is?

## **Changing equilibrium conditions**

Item 7: A system at equilibrium is disturbed by increasing the concentration of NO, <u>immediately</u> after addition of NO, in terms of rate?

Item 9: A system at equilibrium is disturbed by decreasing the volume of the system, <u>immediately</u> after decrease of volume, in terms of rate?

Item 10: Equilibrium is disturbed by decreasing the volume at constant temperature, when <u>new equilibrium is re-established</u>

Item 11: Equilibrium is disturbed by decreasing the volume at constant temperature, when <u>new equilibrium is re-established</u>

A theoretical thematic analysis was helpful in determining the above sub-theme; concentration of reactants and products at equilibrium are equal because equilibrium constant K=1. Prior literature (Canpolat et al, 2006; Hackling & Garnett, 1985; Hameed et al, 1993) on student misconception towards chemical equilibrium has repeatedly identified that students determine concentration of reactants and products were equal, because they relate the word equilibrium to being a state of equality. Hence, while coding for the sub-theme, words describing the process of equality was sought out in student responses.

The following screen shot (Figure 4) of a qualitative data presents an example of the theoretical thematic analysis showing the larger theme: characteristics of equilibrium and sub theme: concentration of reactants and products at equilibrium are equal because equilibrium constant K=1. Coded words are shown in the column referred to a concepts (vocabulary). Student quotes are shown as well.

	Theme 2 – Characteristics of Equilibrium						
	Question 3: At equilibrium, in terms of concentration? (N	=15)					
Ν	Sub Themes	Concepts (vocabulary)	Student quotes				
	Theme 3(a)						
6	Concentration of reactants and products is equal because equilibrium constant K=1	Equal, equilibrium means equal, equalize, same amount, equal means equal concentrations,	<ul> <li>S: "because it talks about their constant over time and they are always going to be same, but sometimes it's going to fluctuate, it's not going to be same thing, the entire time"</li> <li>S: "Equalize the reaction, hence equilibrium"</li> <li>S: "Because K =1, mathematically concentration of reactants and products are equal, it's kind of the purpose of equilibrium"</li> </ul>				

Figure 4: A representative sample of the assessment tool developed for the study to assess qualitative data.

Table 2 below summarizes all the sub-themes that were identified in the current dissertation study. A theoretical thematic analysis was used towards identifying the sub-themes. The sub-themes identified were part of one of the four larger themes identified. The sub-themes are essentially distractors used in the CEMT instrument.

#	Major sub-themes Idenitified through qualitative data
1	As the system approaches equilibrium, Rate of forward reaction increases
2	As the system approaches equilibrium, Reverse reaction is same as forward reaction rate
3	As the system approaches equilibrium, concentration of reactants and products are equal
4	At equilibrium, concentration of reactants and products are equal
5	At equilibrium, rates are equal but not constant
6	At equilibrium, concentration of NO and NOCI are equal
7	At equilibrium, concentration of reactants and products fluctuate
8	At equilibrium K =1 so concentration of reactants and products are equal
9	At equilibrium K<1, total moles of products less than total moles of reactants
10	At equilibrum K =1, so rates and concentration are equal
11	After addition of NO, initially, rate of forward reaction increase and reverse reaction decrease
12	After addition of NO, initially, rate of reverse reaction increase
13	After addition of NO, when equilibrium is re-established, K will be greater
14	After addition of NO, when equilibrium is re-established, K will be less
15	When volume is decreased to a system at equilibrium, initially, rate of forward reaction increase and reverse reaction decrease
16	When volume is decreased to a system at equilibrium, initially, rate of reverse reaction increase
17	When volume is decreased to a system at equilibrium, initially, rate of forward reaction increase and reverse reaction decrease, forward rate greater than reverse rate
18	When volume is decreased to a system at equilibrium, when equilibrium re-established, rate of forward and reverse reactions are equal as initial equilibrium
19	When volume is decreased to a system at equilibrium, when equilibrium is re-established, concentration of NO and Cl2 will be greater in the new equilibrium compared to initial equilibrium
20	When volume is decreased to a system at equilibrium, when equilibrium is re-established, concentration of NO will be greater, C12 will be less
21	When volume is decreased to a system at equilibrium, when equilibrium is re-established, concentration of NO will be less, Cl2 will be greater

Another piece of qualitative data in the data corpus was the simulation notes provided by the students. The simulation notes allowed the researcher to identify to what aspect of the simulation students found most useful. In other words, did students find the audio or visual component more helpful or other components of the simulation. It was evident from post-interview responses that several participants found the visual aspect of the simulation more helfpul over the audio aspect of the simulation.

The chapter described the quantitative and qualitative methodology, research design, research hypotheses, population, sample and instrument to be used in the study.

In the following chapters (Chapter 4 and 5) data analysis, results and findings will be presented.

## CHAPTER IV. DATA, ANALYSIS & RESULTS

#### **Dissertation Study Results**

The purpose of this study was to evaluate the effectiveness of visualization tools such as simulations towards conceptual understanding of chemical equilibrium at the particulate level (microscopic) by students' at the post-secondary level. The study also to seek to understand if students participated in the study held common misconceptions reported in the literature or in addition have students developed newer misconceptions and what thought process guide a student to seek a particular answer choice on the quantitative instrument. The quantitative instrument used in the study was developed to reflect common misconceptions reported in the literature.

To achieve the overall purpose of the study, the following research questions were put forward. They are

- a) What are students' conceptual understandings of chemical equilibrium before interacting with the simulations?
- b) What key characteristics of students' mental model regarding chemical equilibrium concepts can be extracted from student writings, drawings and oral explanation before and after viewing simulations?
- c) What evidence is observed to suggest changes in students' mental models on chemical equilibrium after they use the chemical equilibrium simulations?
- d) What are students' conceptions of chemical equilibrium after interacting with the simulations?

Results of the quantitative and qualitative analysis from the control group will be presented first followed by results of the quantitative and qualitative analysis from the experimental group. A discussion summarizing the findings was presented in the final chapter (Summary and Conclusions).

#### Validity

The CEMT instrument used in the dissertation study was designed around four major themes. The themes are: a) approaching equilibrium (items 1 and 2), b) characteristics of equilibrium (item 3, 4 and 5), c) equilibrium constant (item 6 and 8) and d) changing equilibrium conditions (item 7, 9, 10 and 11). The major themes were identified based on prior research on chemical equilibrium misconceptions (Canpolat et al, 2006; Hackling & Garnett, 1985; Hameed et al, 1993).

## **Face validity**

Face validity was established by consulting faculty who teach the class containing the students sampled for the study.

#### **Demographics**

Students were sampled from three sections of introductory level general chemistry courses at the University of Kentucky. Demographics of students who participated in the experimetal and control group are shown in Table 3. A total of 30 students signed up to participate in the study. Students were randomly assigned to the control and experimental groups. 15 student made up the experimental group, while only 12 student made up the control group. Students' majors were not considered as a variable in the study, hence data on major were not obtained. However during interviews, students informed their majors.

Participant Demographics							
Nu	Number and Percentage of Participants						
Group	Group Caucasian African Hispanic Asian						
American							
Control	10 (83.3%)	0(0%)	0(0%)	2(16.7%)			
Experimental							

Table 3: Demographics of participants who were part of the sample in the experimental group of the study

#### **Construct validity**

Conditional probability represents the chance that one event will occur given that a second event has already occurred (Voska, 1998). Conditional probability allows a researcher to examine how different treatments (cause) had influenced the outcome (effect). Conditional probability analysis was used to determine the relatedness of student reasoning from the semi-structured interview to the answer choice they chose on the CEMT. If intervention is considered as a condition or the cause, then the effect estimated is an increase in the number of participants selecting a correct answer choice.

The five major conditions chosen to correlate student reasoning and their answer choice are as follows a) correct answer provided with correct scientific reasoning (CACR), b) correct answer provided with incorrect scientific reasoning (CAIR), c) incorrect answer provided with incorrect scientific reasoning (IAIR), d) incorrect answer provided with correct scientific reasoning (IACR), and e) correct answer provided with no recorded response (CANR).

Conditional probabilities were determined for the control and experimental group (pre and post quantiative/qualitative data) and comparison will be made between the post conditional probabilities for the control and the experimental group. Comparison were made to determine a) if there was a pattern when a student choose an incorrect answer with an incorrect reasoning for one item also choose an incorrect answer and reasoning for a second item pre-intervention and b) if there was a pattern towards a student choosing a correct answer with a correct reasoning post-intervention.

A coding matrix was generated for pre-quantiative/qualitative and post quantiative/qualitative for both control and experimental groups. The matrices can be found in Appendix D. Conditional probability was performed using the Crosstabs option SPSS. The SPSS output for pre- quantitative/qualitative and post-quantitative/qualitative for control and experimental groups are shown in Table 4, 5, 6 and 7 respectively. The timeline when the dissertation study took place, members of both control and experimental groups have already completed their mid-term test on the topic of chemical equilibrium. Hence, students' experience learning the topic was a contributing.

In the succeding paragraphs, discussion will be provided comparing conditional probability results between the control and the experimental group on the pre and posttest.

In alignment with the literature on common student misconceptions held towards chemical equilibrium concepts discussed in Canpolat et al, 2006; Hackling & Garnett, 1985; Hameed et al, 1993), it is not suprising that a greater proportion of students in both groups fell under the IAIR category (Table 4 and 5). As pointed out in the instrument section (p. 92), items are grouped according under larger themes. Comparing pre quantiative/qualitaive conditional probability data between the control (Table 4) and experimental group (Table 5), following observations were made. In the CACR category,

except for items 2 and 3, the percentage of participants in both groups matched similar in their abilities towards answering a question correctly with a correct reasoning (CACR). Item 3 is a critical one, as it reinforces the idea of a system at equilibrium.

Another aspect that was evident from Table 4 and 5 was students who did not answer items 7 or 9 did not perform well on items 10 and 11 well. Items 7, 9, 10 and 11 assess students understanding of how changing equilibrium conditions affect the reaction rate and concentration of species involved when equilibrium is re-established.

It is evident from Table 6, higher percentag of students in the control group held misconception towards items 1, 5, 7, 9, 10 & 11. If a student has answered all four items or a combination of items (7, 9, 10 and 11) incorrectly, then it is anticipated that the condition (intervention) will allow a student to answer all four items or combination of items correctly. Answering items (1, 2, 3, 4, 5, 6 and 8) correctly with a correct reasoning does not automatically render a student to answer items (7, 9, 10 and 11) correctly. In other words, a student must incorporate additional concepts in to their thought process to answer items (7, 9, 10 and 11) correctly. The assumption is, the intervention is able to provide the necessary scaffolding visually, that would allow students to answer these items correctly.

Item 10 was another interesting case. A smaller percentage of students in the experimental group provided correct answer and a concurrent correct reasoning, while none in the control group answered item 10 correctly. Item 6 remained a special case throughout the study. The only item towards which participants of both groups showed no significant difference in their understanding of the concept of equilibrium constant, even though many participants showed improvement on related items (item 3, 5 and 8). Higher percentage of participants in both groups felt under th IAIR category for items 3, 5, 8, 10

and 11. Item 3 demonstrated the classic case, where students demonstrated the misconception through their reasoning that, at equilibrium concentration of reactant and products has to be equal.

Table 4: Conditional probability output generated using cross tab analysis of the pre-test data in SPSS representing the number of students assigned to the control group

% with	nin Item					
		Students				
		CACR	CAIR	IAIR	CANR	Total
Item	item1	8.3%		75.0%	16.7%	100.0%
	item2	16.7%		66.7%	16.7%	100.0%
	item3	8.3%		75.0%	16.7%	100.0%
	item4			50.0%	50.0%	100.0%
	item5	8.3%		75.0%	16.7%	100.0%
	item6	8.3%		66.7%	25.0%	100.0%
	item7			83.3%	16.7%	100.0%
	item8	16.7%		50.0%	33.3%	100.0%
	item9	8.3%		83.3%	8.3%	100.0%
	item10			100.0%		100.0%
	item11		8.3%	83.3%	8.3%	100.0%
Total		6.8%	0.8%	73.5%	18.9%	100.0%

Item \* Students Crosstabulation

Table 5: Conditional probability output generated using cross tab analysis of the pre-test data in SPSS representing the number of students assigned to the experimental group

Item	* Students	Crosstal	bulation
------	------------	----------	----------

		Students				
		CACR	CAIR	IAIR	CANR	Total
Item	item 1	6.7%		73.3%	20.0%	100.0%
	item2	40.0%		46.7%	13.3%	100.0%
	item3	40.0%		40.0%	20.0%	100.0%
	item4	6.7%		46.7%	46.7%	100.0%
	item5	20.0%		80.0%		100.0%
	item6			86.7%	13.3%	100.0%
	item7	6.7%		93.3%		100.0%
	item8	20.0%		33.3%	46.7%	100.0%
	item9	6.7%		93.3%		100.0%
	item10	20.0%		80.0%		100.0%
	item11	6.7%	33.3%	46.7%	13.3%	100.0%
Total		15.8%	3.0%	65.5%	15.8%	100.0%

% within Item

Evaluting Tables 6 it is evident that despite the fact students were allowed to use their own class notes or textbook on the topic of chemical equilibrium, the percentage of students in the category CACR and IAIR appear very similar. In otherwords, students either had a similar reasoning or an incorrect reasoning between the pre and post-test. In sharp contrast, evaluating Table 7, it is evident that the probability of students falling holding correct scientific reasoning to answer items 1, 3, 5, 10 and 11 correctly has sharply increased.

Table 6: Conditional probability output generated using cross tab analysis of the post-testdata in SPSS representing the number of students assigned to the control group

		Students				
		CACR	CAIR	IAIR	CANR	Total
Item	item1	16.7%		83.3%		100.0%
	item2	25.0%		75.0%		100.0%
	item3	8.3%		75.0%	16.7%	100.0%
	item4	16.7%		58.3%	25.0%	100.0%
	item5	8.3%		91.7%		100.0%
	item6	8.3%		75.0%	16.7%	100.0%
	item7	8.3%		66.7%	25.0%	100.0%
	item8	16.7%	8.3%	75.0%		100.0%
	item9	25.0%		75.0%		100.0%
	item10			100.0%		100.0%
	item11	16.7%		75.0%	8.3%	100.0%
Total		13.6%	0.8%	77.3%	8.3%	100.0%

Item \* Students Crosstabulation

% within Item

Table 7: Conditional probability output generated using cross tab analysis of the post-test data in SPSS representing the number of students assigned to the experimental group

Item * Students Cro.	sstabulation
----------------------	--------------

		Students			
		CACR	IAIR	CANR	Total
Item	item1	33.3%	6.7%	60.0%	100.0%
	item2	40.0%	33.3%	26.7%	100.0%
	item3	40.0%	6.7%	53.3%	100.0%
	item4	53.3%		46.7%	100.0%
	item5	40.0%	33.3%	26.7%	100.0%
	item6	20.0%	46.7%	33.3%	100.0%
	item7	33.3%	53.3%	13.3%	100.0%
	item8	20.0%	46.7%	33.3%	100.0%
	item9	26.7%	53.3%	20.0%	100.0%
	item10	40.0%	13.3%	46.7%	100.0%
	item11	40.0%	40.0%	20.0%	100.0%
Total		35.2%	30.3%	34.5%	100.0%

#### Reliability

Reliability analysis was conducted separately on the pretest and posttest data from the chemical equilibrium assessment instrument. SPSS output of the KR-20 analysis for the pre-and post-test data is shown in Table 8. As suggested earlier, in comparison to the timeline around which the pilot study took place, students had already completed their mid-term examination on the topic of chemical equilibrium. The value of Cronbach's alpha for the pre-test ( $\alpha = 0.44$ ) and post-test ( $\alpha = 0.71$ ) can be seen in Table 8. According to (Devills, 2003; Nunnally, 1994) acceptable values of alpha ranges between 0.7 to 0.95. If alpha is too high, it suggests that some items are redundant. Comparing the pre-tesst and the post-test Cronbach's alpha, there is a sharp increase suggesting that there is more inter-relatedness between items and perhaps the number of items is sufficient.

Table 8: SPSS output of the KR-20 analysis of the pre and post-test data for the controland experimental group

Reliability Statistics				
Test Cronbach's Alpha Number of Items				
Pre-test	0.444	11		
Post-test	0.710	11		

#### **Frequency Analysis**

#### **Pre-Quantative/Qualitative Data Analysis**

Frequency analysis of the pre and post quantiative data along with qualitative data including the theoretical thematic analysis and accompanying student quotes will be present in this section. The pre-test data from the control and experimental groups will be grouped in to a) what common alternative conceptions reported in the literature were held by students in both groups, b) what percentage of students in both groups held additional alternative conceptions identified in the current study and c) what percentage of students in both groups held scientifically acceptable conceptions. The post-test data from the control and experimental groups will be grouped in to a) what percentage of students in both groups retained common alternate conceptions reported in the literature, b) what percentage of students in both groups retained common alternate conceptions reported in the literature, b) what percentage of students in both groups and c) what percentage of students in both groups held correct conceptions alternate conceptions identified in the current study and c) what percentage of students in both groups held correct conceptions and alternate conceptions identified in the current study and c) what percentage of students in both groups held correct conceptions and the findings will be summarized in the final chapter (Summary and Conclusions).

Frequency analysis of the pre-test data representing the common misconceptions held by students in the control and experimental group is shown in Table 9. The percentages are shown inside paranthesis. The first value represent the members of the experimental group and the second value represent the members of the control group. For example, in item 5 (30%, 45%) implies, 30% constitute the percentage of alternative or correct conception held by students in the experimental group and 45% consitute the percentag of alternative or correct conception held by students in control group.

As pointed out earlier in the literature review and the introduction sections, student misconceptions have been reported widely in the literature (Wheeler & Kass, 1978; Hackling & Garnett, 1985; Banerjee, 1991; Huddle & Pillay, 1996; Voska & Heikkinen, 2000). While the above research studies have all addressed chemical equilibrium misconceptions, percentages of misconceptions reported in table 10 were only used from studies conducted by (Hackling & Garnett, 1985; Hameed et al, 1993; Canpolat et al, 2006), as only these three studies have considered the chemical reaction addressed in the study. Percentage of common misconceptions reported in the literature are also shown in the table.

A greater proportion of students held common misconception reported in the literature towards items 1 (27%, 42%), item 3 (27%, 33%), item 5 (40%, 50%), item 8 (87%, 25%) and item 10 (60%, 25%). The most common of all chemical equilibrium misconception reported in the literature is the fact, students carry the notion that at equilibrium, concentration of reactants and products are equal (item 3 and 5). Items 3 and 5 are part of the larger theme, characteristics of chemical equilibrium.

The concept of chemical equilibrium is known to students attending chemistry classes and for which they have a preconception. The preconception of *equilibrium* stems from the idea used in everyday life, where equilibrium means equality of two sides, stability and static in nature (Schafer, 1984). While systems that reach chemical equilibrium may appear macroscopically stable and static, microscopically the system is dynamic not only because of molecular movement but also because the process of bond breakage and creation goes on. Gussarsky and Gorodetsky (1990) explained applying macroscopic qualities to the microscopic level leads to misconception towards

understanding of chemical equilibrium. Hackling and Garnett (1985) reported that students held a simple arithmetic relationship between the concentration of reactants and products. Berquist (1989) reported that students often selected multiple choice answer on an examination dealing with chemical equilibrium without a corresponding level of understanding for the underlying concepts.

Table 9: Frequency analysis of common misconceptions held by students in the control (C) and experimental (E) group on the pre-test data

Category	Misconeption % (C) (N=12)	Misconeption % (EG) (N=15)	Misconception % (Lit)
Approaching equilibrium			
As the reaction approach equilibrium, rate of forward reaction is same as reverse reaction	42	27	17 <sup>b</sup> , 27 <sup>c</sup>
Characteristics of equilibrium			
At equilibrium, concentration of reactants and products are equal	33	27	33°, 57ª
At equilibrium, concentration of NO and NOCl are equal	50	40	53°
At equilibrium concentration of reactants and products are fluctuating	8	20	70 <sup>c</sup>
Equilibrium constant			
After addition of NO and equilibrium re- established, K will be greater	40	33	20 <sup>b</sup> ,
Changing equilibrium conditions			
After addition of NO initially, rate of forward reaction increase and reverse reaction decrease	25	87	43 <sup>b</sup> , 73 <sup>c</sup> , 63 <sup>a</sup>
When volume is decreased to a system at equilibrium, initially, rate of forward reaction increase and reverse reaction decrease	33	47	63 <sup>b</sup> , 50 <sup>c</sup> ,
When volume is decreased to a system at equilibrium, when equilibrium re- established, rate of forward reverse reaction increase, reverse reaction decrease	25	60	67 <sup>c</sup> , 55 <sup>a</sup> , 27 <sup>b</sup>

a:Canpolat et al, 2006; b: Hackling & Garnett, 1985; c: Hameed et al, 1993

A group of students also held the misconception that at equilibrium concentration of reactants and products are equal, based their reasoning around the equilibrium constant (K). Equilibrium constant (K) is measured as the ratio of concentration of products over concentration of reactants. Textbooks or classroom instruction typically reinforce the idea, a system is at equilibrium when K = 1. While K = 1 indicates a system at equilibrium, it does not mean the ratio of products and reactants concentration are equal. In other words, K=1 is simply a symbolic representation of a system at equilibrium. However, students who interpreted K=1 has more than a symbol, took the stance that K=1 implies numerator and denominator must be equal. Hence, concentration of

As noted earlier in the qualitative data section in Chapter III, a deductive or theoretical thematic analysis was used to analyze pre and post-qualitative data. Deductive or theoretical involves coding the data to fit it in to a pre-existing coding frame or the researcher's analytical perceptions. The four larger themes are: a) approaching equilibrium (items 1 and 2), b) characteristics of equilibrium (item 3, 4 and 5), c) equilibrium constant (item 6 and 8) and d) changing equilibrium conditions (item 7, 9, 10 and 11). The major themes were identified based on prior research on chemical equilibrium misconceptions (Canpolat et al, 2006; Hackling & Garnett, 1985; Hameed et al, 1993). Because the CEMT instrument developed for the study was grounded on prior research, distractors (answer choices) for each item contained in the CEMT served as sub-themes. Hence, during theoretical thematic analysis coding was purposeful to fit a code in to a pre-existing codin frame (sub-themes). For example, after analyzing the prequalitative data related to item 3 on CEMT, two set of codes were identified. One set of codes reflect the view reported in literature (Type 1), i.e., preconception of *equilibrium* stems from the idea used in everyday life, where equilibrium means equality of two sides. Other set of codes reflect the view reported in the literature (Type 2), i.e., students took a mathematical view over equilibrium constant K=1. While two types of codes were extracted from the transcript, both set of codes point towards the sub-theme, i.e., concentration of reactants and products are equal because K=1. Table 10 and Table 11 below presents the theme, sub-theme, number of participants, codes and student quotes pertaining to item 3 by group.

Table 10: *Theoretical thematic analysis of control group's pre-qualitative data pertaining to item 3* 

	Theme 2 – Characteristics of Equilibrium						
	Question 3: At equilibrium, in terms of a	concen	tration? (N=1:	5)			
Ν	Sub Themes		Concepts (vocabulary)		Student quotes		
	Control group						
	Theme 3(a)						
4	Concentration of reactants and products is equal because equilibrium constant K=1	mean equal equili equal conce	brium, k is	means C10: K =1, equili C11: equili equal	Well, equilibrium s K =1" "I choose A because its equal, so brium" "I thought of brium, so K must be to 1, and hence ntrations must be		

Table 11: *Theoretical thematic analysis of experimental group's pre-qualitative data pertaining to item 3* 

	Theme 2 – Characteristics of Equilibrium						
	Question 3: At equilibrium, in terms of concentration? (N=15)						
Ν	Sub Themes	Codes	Student quotes				
		Experimental group					
	Theme 3(a)						
4	Concentration of reactants and products is equal because equilibrium constant K=1	Type 1 equilibrium means equal, Type 2 Arithmetic, ratio, K=1	<ul> <li>E1: "The concentration of reactants and products equal if K=1 that's what it reads, so when by definition K is equal to 1, when the concentration of products and reactants is the same"</li> <li>E14: "I have kind of remembered that K =1 is the goal to reach for equilibrium, it's like perfect equilibrium I think"</li> <li>E13: "I know, when I was thinking of equal, you know cuz K = 1"</li> </ul>				

50% of students in the control group and 40% of students in the experimental group who answered item #5, held the misconception that concentration of NO and NOCl at equilibrium must be equal because they existed in a 2 to 2 stoichiometry. Bilgin (2006) suggested students learn the taught rule by heart and they try to apply it without understanding, fixating on the pervasive set of reasoning rule-rote recalling algorithm. In particular for items 5, the misconception was found to stem out based on consideration of co-efficients in a chemical reaction. The development of this misconceptions can be attributed to considerable emphasis placed on reaction stoichiometry in introductory topics Hackling and Garnett (1985) and Hameed et al (1994). Unlike how different types

of codes were extracted for item 3, students who held the misconception (concentration of reactants and products are equal because they exist in a 2:2 stoichiometry) for item 5, have incorrectly applied the phenomenon of stoichiometry. This finding concurs with the finding reported by Hackling and Garnett (1985) above. Table 12 presents the thematic analysis of the pre-qualitative data for both groups.

Table 12: *Theoretical thematic analysis of control and experimental group's prequalitative data pertaining to item 5* 

	Question 5: At equilibrium, in terms of stoichiometry? (N=15)				
		Contro	l group		
Ν	Sub Themes	Concepts (vocabulary)	Student quotes		
	Theme 5(a)				
6	Equal amount of NO and NOC1	Arithmetic, equal, stoichiometry	E1: "Cuz, NO and NOCl exists in a 2 to 2 stoichiometry, there will be equal amount of NO and NOCl"		
			<b>E4:</b> "but yeah ,looking at the reaction, the stoichiometry is 2:2, you should say that under certain conditions, it makes sense"		
			<b>E15:</b> "Whenever I looked at the equation, they both 2 in front of them, so it's a 2 to 2 or 1 to 1, so will be equal amounts of them"		

	Experimental group				
Ν	Sub Themes	Concepts (vocabulary)	Student quotes		
	Theme 5(a)				
6	Equal amount of NO and NOC1	2:2 means equal concentration Co-efficients are equal, so concentration is equal	<ul> <li>C1: "so they do have a 2 to 2 stoichiometry, I knew that at equilibrium, C wasn't going to be right, as it doesn't shift, I don't think Cl2 is going to be a limiting reagent, cuz its at equilibrium, I thought B sounded right, as we did ICE table, I remembered using coefficients"</li> <li>C2: "Since it's a 2 to 2 ratio, it makes sense, the amounts go to be equal. So that's why I decide to go with B"</li> <li>C5: "both NO and NOC1 got coefficients of 2, so when equilibrium is attained, they should both be in equal amounts"</li> <li>C12: "I didn't know if it's A or B, because Cl2 is less, so it could be limiting, but I decide to go with B, it's the strongest of the two"</li> </ul>		

40% of students in the control group and 33% of students in the experimental group held a mathematical view and erroneously applied Le Chatelier's and stoichiometric principles while solving item 8. Item 8 expected students to predict whether equilibrium constant would stay the same, increase or decrease, when the concentration of NO is increased at equilibrium. In other words, NO is a reactant, so what happens to the equilibrium constant of a reaction when reactants are added to a system at equilibrium. The common view held by participants was, because more NO is added to the system, the reaction will shift towards the right, because the right side had less moles and hence concentration of NOCl will increase and that of NO and Cl<sub>2</sub> will decrease. Hackling and Garnett (1985) and Hameed et al (1994) reported similar findings in their study. They suggested students in their study focused on changes in NOCl concentration and did not consider the changes in the concentrations to the NO and Cl<sub>2</sub> species. They further added that student's lack of approaching the reaction from a system's perspective could be due to their lack of understanding of the way in which numbers of moles of reactants being consumed and products being formed in a chemical reaction are related. Cheung (2004) described the inadequacy of Le Chatelier's principle towards solving chemical equilibrium problems for the gaseous system  $N_2(g) + H_2(g) \leftarrow 2 NH_3(g)$ . While the system described in this article is different from the system considered in the current study, they share few similarities. They are a) both systems attain chemical equilibrium, b) both systems have gaseous reactant and product species and c) both systems have different reactant to product stoichiometric ratio. If the concentration of  $N_2$ (g) is increased in the chemical system shown above, Chueng (2004) suggested mechanical application of Le Chatelier's principle (LCP) would suggest the equilibrium

position would shift to right. However, addition of  $N_2$  (g) will increase the total volume of the system. The addition of  $N_2$  (g) also increases the partial pressure of  $N_2$  (g), while the partial pressure of  $H_2$  (g) will decrease. Unfortunately LCP cannot give a definite prediction to determine whether equilibrium shift towards right or left will predominate. The reasoning suggested by Cheung (2004) supports the view that incorrect application of LCP can lead to incorrect answers. Cheung (2009) further emphasized that chemistry teacher educators, textbook writers, school teachers must be educated on the inadequacy of LCP. The reason being, classroom instruction pertaining chemical equilibrium involving LCP, often expect students to predict the direction of equilibrium shift. Majority of textbooks even provide a table listing the direction of equilibrium shift using LCP, when a system at equilibrium is altered. Instruction does not focus on what happens to the system when it re-attains equilibrium. Rather the instruction focuses on direction of equilibrium shift. Providing students with a table that lists equilibrium shifts under different conditions, incorporates an algorithmic view in the minds of students. Students in both the control and experimental demonstrated such an algorithmic view about equilibrium shift. It was evident through pre-qualitative interviews from students in both groups (experimental n = 5 and control n = 3). The 8 participants held either a mathematical view or incorrectly applied LCP to solve the problem. The finding concur with reasons suggested by Cheung (1999 & 2004). Table 13 presents the thematic analysis of the pre-qualitative data depicting control and experimental group participant's response to item 8.

# Table 13: *Theoretical thematic analysis of control and experimental group's prequalitative data pertaining to item* 8

<u> </u>	Question 8: After addition of [NO], when new equilibrium is re-established? (N=15) Experimental group					
	C 1 71	0.1				
N	Sub Themes	Cod	es	Student quotes		
	Theme 8(a)					
5	Equilibrium constant greater than 1	Arithmetic, ratio, more versus less, co- efficients, prior knowledge		E3: "I was still thinking of the 1 to 1 ratio, since we are adding more, it can now become a 2 to 2 or even a 3 to 3 ratio? It's still the same, its just a lot greater than before"		
				<ul> <li>E14: "I was thinking, trying to remember prior knowledge, about what we learned in class, we learned a few tricks, like, more products added, the K go this way, whatever and took a guess, if you add more reactants, it shifts to the products"</li> <li>E4: "the concentration of NOC1 is going to be</li> </ul>		
				greater in the newer equilibrium, so your concentration of the products will be higher, and reactants will be lower, so that would create a bigger constant K"		
ľ			Cor	ntrol group		
Ν	Sub Themes		Codes	Student quotes		
	Theme 8(a)					
3	1		More over less, Arithmetic vs ratio	<b>C8:</b> "I choose B, addition of NO will make the constant greater"		
				<b>C10:</b> "I decide to go with B, because when you add NO, the equilibrium will shift to right, so you'll have more of NOC1, so according to the K expression, K will be greater"		

The last item that I would like to address before addressing additional

misconceptions is item 9. 33 % of students in the control group and 47% of students in the control group held the common misconception, i.e., when a system at equilibrium is disturbed by a decrease in the volume of the system, rate of the forward reaction increases and rate of the reverse reaction decreases. Hackling and Garnett (1985) suggested a possible reason behind this misconception. The misconception was caused by students believing that reaction rates adjusted to facilitate the predictions made using LCP. Similar findings was reported by Cheung (2004). While the participants were teachers and the chemical system considered was different than the one considered in the current study, the findings concur with reasoning suggested by Hackling and Garnett (1985). More than 50% of teachers who participated incorrectly applied LCP to make predictions about the reaction rate when the volume of a system is decreased. Only 2 out of the 33 had valid scientific reasoning behind their answer choice.

The follow interview responses concurs with the reasoning suggested by Hackling and Garnett (1985). The participants have clearly applied LCP to make predictions about the reaction rate. While the students were able to understand the relationship between pressure and volume, the understanding was not extended to relate volume to molar concentration. Following is the conversation between the researcher and the student (R corresponds to Researcher and P corresponds to Participant.

## Experimental group

*P*: *Ummm*, [long pause], well I had to think about this one

*R:* No problem, take your time

*P:* Well, you decrease volume, so you increase pressure, so it will move to right, so reaction cannot move to left, so, it's like, the, the forward should increase and reverse should decrease

**R**: You mean the rate?

**P:** Yeah that's what I meant

R: Thanks

## Control group

**R:** Going to #9, what was your reasoning?

*P: I know when volume decreases pressure decreases, and there is 3moles on the reactant side and 2 moles on the product side and its gonna wanna go to the side with less moles, so I knew that the forward reaction was going to increase and the reverse reaction was going to decrease, so I picked C* 

It is evident from the above responses, the students begins by correctly explaining the relationship between pressure and volume, but failed to extend the relationship between volume of the system and molar concentration. It is to be noted rate of a reaction is ratio of the change in molar concentration over change in time. Both participants have used the concept of moles from a purely mathematical and logical (application of LCP) perspective without understanding the relationship between moles and volume (molar concentration).

Theoretical thematic analysis is shown below in Table 14. Members of both groups who held similar misconception towards item 9, i.e., rate of forward reaction increases and rate of reverse reaction decreases had similar reasons. It is evident from the codes column in Table 14, codes were similar among the 11 participants. In other words, all 11 participants held the common view suggested by Hackling and Garnett (1985), i.e., students' prediction of rates were therefore based on a knowledge of the expected changes in equilibrium concentrations determined from application of LCP.

Table 14: Theoretical thematic analysis of pre-qualitative data containing commonmisconceptions held by control and experimental group towards item 9

	<b>Question 9:</b> Equilibrium is disturbed by decreasing the volume at constant temperature, initially? (N=15)				
Ν	Sub Themes	Concepts (vocabulary)	Student quotes		
	•	Experin	nental group		
	Theme 9(a)				
7	Rates of forward reaction increase, reverse reaction decrease	More vs less moles, Increase pressure vs decrease volume,	<ul> <li>E7: "Like I said if you decrease or constrain volume, its going to favor the side with least moles, so the forward reaction will increase and the reverse reaction will decrease"</li> <li>E9: "Well, you decrease volume, so you</li> </ul>		
			increase pressure, so it will move to right, so reaction cannot move to left, so, it's like, the, the forward should increase and reverse should decrease		

Ν	Sub Themes	Codes	Student quotes			
	Control group					
	Theme 9(a)					
4	Rates of forward reaction increase, reverse reaction decrease	Volume vs pressure, more vs less moles	<b>C1:</b> "I know when volume decreases pressure decreases, and there is 3moles on the reactant side and 2 moles on the product side and its gonna wanna go to the side with less moles, so I knew that the forward reaction was going to increase and the reverse reaction was going to decrease, so I picked C"			

Additional misconceptions were distractors that were purposefully included in the CEMT under each item. The reasons were a) research studies on chemical equilibrium misconceptions have focused on the rate aspect while a system approaches equilibrium but did not take in to account the concentration aspect, b) studies that have looked in to student misconception on chemical equilibrium have suggested, students incorrectly apply stoichiometric principles, but failed to quantify the misconception and c) research

studies on chemical equilibrium misconceptions have repeatedly identified that students hold an algorithmic reasoning towards solving chemical equilibrium problems.

Additional misconceptions held by students in both control and experimental group is shown in Table 15. In line with the reasons on why additional misconceptions were identified, the items towards which students had higher percentage of additional misconceptions include items 6, 9 and 11. 33% of participants in both groups who answered item 6, held the misconception that equilibrium constant K will be less than 1. While a total of 9 participants picked this choice on the CEMT, it was only possible to obtain 2 participants response to this item. The major reason being time constraint. Thematic analysis of student's additional misconception towards item 9 is shown in Table 16. It was evident from the transcribed responses, the codes were very similar and they point towards the common sub-theme, i.e., equilibrium constant K is less than 1. The primary reason being students' answer choice was there are 2moles of NOC1 (products) compared to 3 total moles of NO and Cl<sub>2</sub> (reactants). It is evident from the response, that students held a weaker understanding of the concept of moles. They have incorrectly applied stoichiometric co-efficients in place of molar concentration.

Table 15: Frequency analysis of additional misconceptions held by students in the control (C) and experimental (E) group on the pre-test data. (NA = not applicable)

Category	Misconception	Misconception
	%	%
	(C) (N=12)	(E) (N=15)
Approaching equilibrium		
Rate of forward reaction decrease at the same rate	25	20
as the reverse reaction		
Rate of forward reaction increase	17	NA
Concentration of reactants and products are equal	25	20
Concentration of reactants 3 times more than	25	20
concentration of products		
Concentration of reactants and products is	33	NA
constant because K<1		
Characterisitics of equilibrium		
Concentration of products is greater, because K>1	17	NA
Because Cl2 is a limiting reagent, there will be no	25	NA
Cl2 left		
Equilibrium constant		
At equilibrium, K is less than 1, because total	33	33
moles of products is less		
At equilibrium, $K = 1$ , because concentration of	8	27
reactants and products are equal		
Changing equilibrium conditions		
At equilibrium, when concentration of NO is	8	NA
increased, initially, rate of forward reaction will		
not change, because volume is kept constant		
When volume is decreased to a system at	25	20
equilibrium, initially, rate of reverse reaction		
decrease		
When volume is decreased to a system at	42	NA
equilibrium, when equilibrium is re-established		
rate of reverse reaction increase		
When volume is decreased to a system at	42	67
equilibrium, when equilibrium is re-established,		
concentration of NO Cl2 will be lesser and NOCl		
will be greater than the initial equilibrium		

Table 16: *Theoretical thematic analysis of pre-qualitative data containing additional misconceptions held by control and experimental group towards item 9* 

	Theme 3 – Equilibrium Constant			
	Question 6: At equilibr	ium, what is true about	equilibrium constant?(N=15)	
		Experimental	group	
Ν	Sub Themes	Concepts (vocabulary)	Student quotes	
	Theme 6(a)			
5	Equilibrium constant (K) is less than 1	Arithmetic application,	E15: "because there is two moles of products and 3 moles of reactants, so K must be less than 1"	

	Control group					
Ν	Sub Themes	Codes	Student quotes			
	Theme 6(a)					
4	Equilibrium constant (K) is less than 1	Arithmetic application, Knowledgeable guess	<b>C1:</b> "I kinda forgot what K was, a little bit, I do remember it was products over reactants, and I knew that it would be NOC1 squared over NO squared and C12. I kind guessed it to be less than 1, I just wasn't sure there either. I guessed products will be less than reactants"			

25% of students in the control group and 20% of students in the experimental held the additional misconception towards item 9, i.e., rate of reverse reaction decrease as the volume of the system is lowered. Unfortunately, participant's response were not recorded for this misconception. While this misconception was not reported in prior research on chemical equilibrium misconception studies, an alternative statement suggested by Hackling and Garnett (1985) could be used to explain student reasoning behind their choices. According to Hackling and Garnett (1985), students generally had a qualitative understanding of the way in which the concentration of reactants and products changed as the reaction approached equilibrium. The misconception may result from students' prior experience with chemical reactions which do in fact show an increase in rate as the reaction takes place. For example when a piece of magnesium (Mg) ribbon is placed in dilute acid, resulting in rapid evolution of hydrogen gas. In these reactions, there are special factors that govern the increase in rate of a forward reaction. It is likely, students do not develop complete understanding of these special factors, but instead develop the misconception that the rate of a chemical reaction increases as the reaction proceed towards equilibrium. Because students have developed the misconception, rate of a reaction increases, they believe the opposite is true, i.e., rate of reverse reaction decreases. This misconception is further reinforced by misapplication of Le Chatelier's principle. Because classroom instruction continue to reinforce the idea, when the volume of a system is reduced the reaction would shift to the side with least moles (LCP), students associate the equilibrium shift with rate of a reaction.

Finally item 11 is a classic case of misapplication of Le Chatelier's principle. 42% of students in the control group and 67% of students in the experimental group held the misconception that when volume is decreased to a system at equilibrium, when equilibrium is re-established, concentration of NO Cl2 will be lesser and NOCl will be greater than the initial equilibrium. The reasoning suggested by Cheung (2004) supports the view that incorrect application of LCP can lead to incorrect answers. Cheung (2009) further emphasized that chemistry teacher educators, textbook writers, school teachers must be educated on the inadequacy of LCP. The reason being, classroom instruction pertaining chemical equilibrium involving LCP, often expect students to predict the direction of equilibrium shift. Majority of textbooks even provide a table listing the

direction of equilibrium shift using LCP, when a system at equilibrium is altered. Instruction does not focus on what happens to the system when it re-attains equilibrium.

Rather the instruction focuses on direction of equilibrium shift. Providing students with a table that lists equilibrium shifts under different conditions, incorporates an algorithmic view in the minds of students. Students in both the control and experimental demonstrated a combination of algorithmic view and misapplication of LCP while answering the item. Thematic analysis of student's misconception over item 11 is shown in Table 17.

Table 17: *Theoretical thematic analysis of pre-qualitative data containing additional misconceptions held by control and experimental group towards item 11* 

	Question 11: Equilibrium is disturbed by decreasing the volume at constant temperature, when new equilibrium is re-established (concentration) (N=15) Experimental group				
Ν	Sub Themes	Concepts (vocabulary)	Student quotes		
	Theme 11(a)				
10	Concentration of NO and C12 will be less and NOCl will be greater in the newer equilibrium	Le Chatelier's principle, algorithmic, guess work, process of elimination	E1: "So you go to the side with the least amount of stress, so we go to right, going to (d), we have the concentration of C12 will be less than first, and the concentration of NOC1 would have to increase as in (e)" E13: "Umm, there's less concentration of some of these, so I choose b & d which is less and then I am not sure with e, I guess it's gotta be greater"		

	Control group					
Ν	Sub Themes	Codes	Student quotes			
	Theme 11(a)					
5	Concentration of NO and Cl2 will be less and NOCl will be greater in the newer equilibrium	Le Chatelier's principle, algorithmic, guess work,	C1: "Decrease volume means increase pressure, 3 moles on the reactant side and 2 moles on the product side, it's gonna shift to the side with less moles, and I know that the reaction is going to shift to the right, to decrease the pressure, the NO and C12 would decrease and NOC1 would increase" C3: "Well if you decrease the volume, you go			
			towards the side with less amount of gas, and that was on the right side. So equilibrium will shift towards right, and I selected choices that fitted the logic. That's how I ended up with a, d & e" C4: "I wasn't entirely sure, I just went off with the strongest choice possible, I used Le Chatelier's principle to make my decision"			

Comparing the codes obtained from the control and experimental group, it is quite obvious they appear similar. The reason being students in both groups applied LCP. A representative transcribed response below describe misapplication of LCP.

**R:** okay, let's go with #11, the system is at equilibrium right? And you disturb it by decreasing volume, equilibrium has to re-establish right? Cuz all reversible reactions eventually has to get back to equilibrium right? So why you choose a, d and e?

*P*: okay (a) reads concentration of NO will be less than the first equilibrium. Okay when we take away volume, we got lot of this NO and Cl2, actually you got 2 NO's and one Cl2, these take up more space collectively than NOCl would, so if we decrease the volume, in order to relieve the most amount of stress on the system, we have to take away, we want to put, we want to have the same amount of products. So you go to the side with the least amount of stress, so we go to right, going to (d), we have the concentration of Cl2 will be less than first, and the concentration of NOCl would have to increase as in (e).

While the above student response with respect to item 11 has elements of scientific reasoning such as decrease in volume will lead to an increase in pressure, the scientific reasoning becomes weak as soon as the student switched over towards a mathematical or algorithmic application of LCP towards solving the problem.

The succeeding paragraphs would present analysis of correct responses provided by students on the pre-test. A correct response does not imply the student had a corresponding correct reasoning. Table 18 presents correct responses held by participants in both groups. Items 3, 4, 5 and 8 were answered correctly by higher percentage of students. It is worthwhile to look at representative student responses during the prequalitative interview phase from both groups.

For item 3, 42% of students in the control group and 60% of students in the

experimental group had correct responses.

Table 18: Frequency analysis of correct responses held by students in the control (C) and experimental (E) group on the pre-test data.

Item	Category	Correct % (C) (N=12)	Correct % (E) (N=15)
	Approaching equilibrium		
1	Rate of forward reaction decrease as the reaction gets going	25	33
2	None of the above	17	53
	Characteristics of equilibrium		
3	Concentration of reactants and products constant over time	42	60
4	Forward and reverse reactions continue to occur, rates of forward and reverse reactions are equal and rates are constant over time	50	53
5	None of the above	67	20
	Equilibrium constant		
6	Equilibrium constant K =1, rates of forward and reverse reactions are equal	33	13
8	After addition of NO to a system at equilibrium and when equilibrium is re-established, equilibrium constant K is the same as before	50	67
	Changing equilibrium conditions		
7	After addition of NO initially, rate of forward reaction will instantenously increase	17	7
9	When volume is decreased to a system at equilibrium, initially, rate of forward and reverse reaction increase	0	13
10	When volume is decreased to a system at equilibrium, when equilibrium is re-established, rate of forward and reverse reactions are equal and greater than initial equilibrium	0	20
11	When volume is decreased to a system at equilibrium, when equilibrium is re-established concentration of NO, Cl2 and NOCl will be greater than the initial equilibrium	17	27

Due to time constraints, it was not possible to record each participant's response.

However, a few participants response were recorded. Below is a comparison between two

student responses. The first response came from a student in the experimental group and the second response came from a student in the control group.

#### Experimental group

**R**: So same with #3, why did you go with (c) why is that?

*P:* Well, Ummm, concentration of reactants and products is constant over time, Ummm, equilibrium just means that, both forward and reverse reactions are happening at the same rate. So, the concentrations don't change otherwise manipulated, if left alone it will stay the same at equilibrium

The above response suggests that, the student had a valid scientific reasoning on why at equilibrium concentrations are constant and remain unchanged.

### Control group

**R**: So why did you decide to go with c for #3?

*P:* Ummm, this one was quite obvious, I learned in lecture, that equilibrium concentration is constant, cuz K = 1

**R**: Okay why you think its constant

**P:** Like I said, cuz K = 1 its equilibrium and hence it constant

R: Okay, moving on

In contrast to the earlier response, the student who had the response above did not had a valid scientific reasoning as to why concentration of reactants and products at equilibrium remain constant over time. The student response suggest rote memory at best. Since high score on an examination are generally interpreted by students as an indication that they understood the material. Questions that require students to synthesize information and apply concepts are not very common in such examinations. To demonstrate mastery of chemical equilibrium concepts, for example, students typically asked to solve computational problems; correct results are accepted as an indication that students "understand" equilibrium correctly. Thus, correct responses do not necessarily reveal whether a student understands chemical equilibrium but only indicate that the student can compute equilibrium constants or calculate equilibrium concentrations. It is likely that such students will assimilate any misunderstandings of chemical equilibrium into their reasoning pattern and thus propagate additional misunderstandings about other chemistry topics. Berquist (1989) found that students often selected the correct multiple choice answer on an examination dealing with chemical equilibrium without a corresponding level of understanding for the underlying concepts. In the above response it is evident the student was successful in recalling information from the lecture, but could not explain why rates are equal and concentration remains constant at equilibrium. Participants in both groups exhibited information recall not just for item 3, but also for other items. Thematic analysis shown in Table 19 describes information recall.

	1				
	Theme 2 – Characteristics of Equilibrium				
	Question 3: At equilibrium, in terms of concentration? (N=15)				
		Contr	ol group		
N	Sub Themes	Concepts (vocabulary)	Student quotes		
	Theme 3(b)				
5	concentrations don't change over time	Remember, recall, rates stay the same, process of elimination	<b>C1:</b> "I remember, I remember, while learning, when you had equilibrium, I just remembered concentration of reactants and products are constant because, the rates were staying the same"		
			C9: "I said C because, neither A or B is correct"		

Table 19: Thematic	analysis of n	pre-aualitative da	ata from the control	group for item 3.
1 4010 191 11000000	childrey bib of p			8. onp jo. none.

As with other items, relatively a smaller number of provided correct reasoning for item 5. Process of elimination was one of the preferred choice among participants throughout the study, especially when they answered an item correctly. The following student response is an example of the process of elimination. Following is a representative interview response from both groups

### Control group

**R**: So, why did you go for d with #5?

*P:* Ummm, [long pause], well, wait, okay, I know, well, A can't be right, as it's at equilibrium, you gotta have some left, 2 to 2 does not mean it had to be equal and it can't fluctuate, so D had to be it.

**R**: Good, you had a good reason behind your elimination

**P:** Yeah, [laughs]

#### Experimental group

**R:** So what was your reasoning behind #5?

*P*: Well, choice A, I guess I didn't feel like I had enough information and C equilibrium shifting doesn't make sense, as equilibrium is shifting, since we are at equilibrium.

The above response suggest, the student has made use of a process of elimination, however the response does suggests a valid scientific reasoning behind the elimination process.

The following paragraphs would focus on discussion about student response to item 11. The following transcribed responses compare two situations; correct answer with correct reasoning and incorrect answer with incorrect reasoning.

### Experimental group

### Correct answer with correct reasoning

*R*: So for #11, you decide to go with b, c and e. why is that?

*P:* Well, Ummm, the concentrations of the substances in the solution are greater, concentration is the measure of the amount of the substance over volume, if volume is lower then concentration must be higher.

*R: Very good, very good.* 

The above response suggest the student had a stronger foundational knowledge. The student was able to relate how decrease in the volume of a system affects the molar concentration of all species contained in the system.

### Control group

# Correct answer with incorrect reasoning

**R**: For #11, b, c & e. what was your reasoning?

*P:* I think I read it as wrong, so if you give me a chance to change, I would change to a different one

*P: I decided why I came up with this answer. Concentration is moles over liter, so if you gonna decrease the volume, the denominator has gone down, so concentration is gonna go up.* 

While the above student had chosen the correct answer choice, the response does not justify his/her stance in choosing the answer choice. In fact, the student switched to an incorrect answer choice on the post-test.

Finally, the following paragraphs provide discussion on student reasoning behind item 8. 50% of students in the control group and 67% of students in the experimental group choose correct choice for item 8, i.e. equilibrium constant K will be the same when equilibrium is re-established. Following is a comparison between student responses. The first response is from a student in the experimental group and the second is from a student in the control group. Since it was not possible to obtain each participant's reasoning behind their answer choice, a participant's response cannot be generalized to explain other participant's reasoning who had a similar answer choice. The purpose behind participant's response discussion is to establish connectivity between the responses to findings in the literature. In the responses below it is evident the student was able to narrow down the correct answer, however the student did not have a valid reasoning. As pointed out by Berquist () students often selected the correct multiple choice answer on an examination dealing with chemical equilibrium without a corresponding level of understanding for the underlying concepts.

### Experimental group

#### Correct answer but invalid reasoning

**R:** Why did you decide to go with (a) for #8?

P: This is the opposite of what I just said. As far as

*P:* I know, I mean the initial concentration does not affect K, so that's why I picked that one.

**R**: What do you mean by initial concentration?

P: I mean adding NO

**R**: Why does it not affect?

P: I guess it just doesn't

**R**: I mean, what I'm getting at is, why you think the initial concentration of NO does not affect?

# P: I am not sure.

In the above response, it is evident the student choose the correct answer, however fell short with the reasoning. The student's reasoning neither does not incorporate explanation on how affecting a component of the system affects other components of the system, i.e., how addition of NO, affects not only the concentration of NO, but also the concentration of NOCl and Cl<sub>2</sub>. It is to be noted, that equilibrium constant will be the same, but concentration of each of the species will be different when equilibrium is re-established.

#### Control group

#### Correct answer but invalid reasoning

**R**: So what was your reasoning behind your answer choice for #8?

P: I decide to go with A for #8, was, because, addition of NO is offset with the heat,

**R**: what you mean by offset with hear?

*P*: I mean the reaction is exothermic

**R**: Okay, how do you think exothermic reaction is important?

**P**: Well in exo, if you had NO, it will go to right

**R:** You mean exothermic?

P: Yeah

**R**: So how does that keep equilibrium constant the same?

**P:** Now that we talk about it, I think I should have gone with B, cuz you will have more products

In the above response, while the student had chosen the correct answer, he/she did not provide valid reasoning to support their answer choice. The student clearly has put in a collection of un-related ideas to answer the question. The question clearly suggested, the temperature of the system is constant. Only if the temperature of a system is altered, it will have an effect on the enthalpy change (heat) of a reaction and the overall equilibrium shift and the equilibrium constant.

In the above paragraphs the pre-quantitative and qualitative data was analyzed. Common misconceptions, additional misconceptions and correct conceptions held by participants in both groups was discussed. In the succeeding section discussion will be based on the post-quantitative and qualitative data analysis.

### Post-Quantative/Qualitative Data Analysis

This section presents the findings from the CEMT posttest results and the analysis of the post-interview responses for experimental and control groups. Participants in the control group were allowed to use their lecture notes prior to commencing the post CEMT assessment. Common misconceptions held by participants in both groups are shown in Table 20.

For item 1 42% of participants in the control group and 7% of the participants in the experimental group held the common misconception, i.e., rate of the forward and reverse reaction remains the same as the system approaches equilibrium. While the percentage of participants in the control group has not changed, the percentage of participants holding the misconception in the control group has gone down from 27% to 7%. Following transcribed response is the reasoning provided by a student in the experimental group post intervention.

*R*: so between the first test and the post-test, your answer choice for #1, stayed the same, what was the reason?

P: I remembered my professor saying, at equilibrium the reaction rates are equal

**R:** This ones approaching remember

**P:** That's what was confusing.

*P:* As it approaches equilibrium, I would say, then, [long pause], I would say that, [long pause], well the forward reaction would increase, cuz you are making products

While the student was able to notice the reaction is approaching equilibrium and was aware of it. Yet the student was incorrectly applying ideas in the wrong context. The primary reason behind such a confusion is partly because, the concept of a system approaching equilibrium is rarely addressed in lectures. Another issue with the student's response is, according to the student rate of the forward reaction would increase. However, rate of the forward reaction should decrease. The student is associating direction of a reaction with what is being made, i.e., the student associate more products formed in the forward reaction to a concurrent increase in rate. Gussarsky and Gorodetsky (1990) explained applying macroscopic qualities to the microscopic level leads to misconception towards understanding of chemical equilibrium. The student is associating matter (ontological category) which was product formed to a process (ontological category) which is rate of a reaction. More discussion about ontological shift will be presented in the discussion section (chapter 5).

For item 3 33% of students in the control group and 7% of students in the experimental group retained the common misconception reported in the literature, i.e., at equilibrium, concentration of reactants and products are equal. While comparing the pretest and post-test data for the common misconception held by participants for item 3, it is evident 33% of students in the control group held the misconception and 27% of students in the experimental group held the common misconception. While there is no difference in the percentage of participants holding this misconception in the control group, only one student (7%) in the experimental group was holding this misconception. It would be worthwhile to look in to participant reasoning from the control and experimental group for item 3.

Table 20: *Frequency analysis of common misconceptions held by students in the control* (*C*) *and experimental* (*E*) *group on the post-test data* 

Category	Misconeptio	Misconeption	Misconception
	n % (C)	% (E)	%
	(N=12)	(N=15)	(Literature)
Approaching equilibrium			
As the reaction approach equilibrium,	42	7	17 <sup>b</sup> , 27 <sup>c</sup>
rate of forward reaction is same as			
reverse reaction			
Characteristics of equilibrium			
At equilibrium, concentration of	33	7	33°, 57 <sup>a</sup>
reactants and products are equal			
At equilibrium, concentration of NO	75	20	53°
and NOCl are equal			
At equilibrium concentration of	NA	0	70 <sup>c</sup>
reactants and products are fluctuating			
Equilibrium constant			
After addition of NO and equilibrium	42	40	20 <sup>b</sup> ,
re-established, K will be greater			
Changing equilibrium conditions			
After addition of NO initially, rate of	25	27	$43^{\rm b}, 73^{\rm c}, 63^{\rm a}$
forward reaction increase and reverse			
reaction decrease			
When volume is decreased to a system	42	27	$63^{\rm b}, 50^{\rm c},$
at equilibrium, initially, rate of forward			
reaction increase and reverse reaction			
decrease			
When volume is decreased to a system	8	0	67 <sup>c</sup> , 55 <sup>a</sup> , 27 <sup>b</sup>
at equilibrium, when equilibrium re-			
established, rate of forward reverse			
reaction increase, reverse reaction			
decrease			

a:Canpolat et al, 2006; b: Hackling & Garnett, 1985; c: Hameed et al, 1993

# Experimental group

# Incorrect answer with incorrect reasoning

*R*: *With #3, no change, why is that* 

*P:* # 3 is one thing, I was not really sure about, I was thinking was, like the equilibrium constant does not necessarily mean, it does not have to do with concentration, its like in relation to each other,

*R*: So you couldn't find any convincing answer from the simulation to answer this one?*P*: yeah, right

It is evident from the response above that the student was unable to extract information from the simulations regarding the characteristic of chemical equilibrium. Every simulation except for simulation #5 emphasized the idea of a chemical equilibrium. Comparative responses from the control group students follow.

### Control group

Incorrect answer with incorrect reasoning

# Response 1

**P**: Well, equilibrium means K = 1

**R**: So that was basically it?

**P:** Yeah it was the definition, well K = Q that's went you reach equilibrium

### Response 2

**R:** So what was your reasoning behind #3?

*P:* On the first test, I choose B, I choose, A because, because of, at equilibrium, they have to be equal, as from the notes, I got the idea K is equal to 1

**R**: so is that you got it from the notes?

**P**: Yeah the notes said a system is at equilibrium when equilibrium equal 1

**R:** So K = 1, means concentration is equal

### **P:** Yes it is

#### Response 3

**R**: so why did you change your answer on the post-test? You had d last time, this time you got a

*P*: on the pre-test I had none of the above, although I was not sure, so I kinda decide to go with d but this time around I put a little more logic in it, I just went with a .

*R*: What logic are you referring to?

*P*: Umm, I mean, the lecture notes suggested, K=1 implies equilibrium

*R*: So, the lecture notes helped you make that decision?

*P*: yeah that's right

In Response 1 above, the student had the correct symbolic definition of a system at equilibrium. Q is typically the term used to refer to an intermittent equilibrium constant, when Q becomes equal to the value of K (original equilibrium constant), the system is defined to have achieved equilibrium. While the symbolic relationship Q = K, characterizes a system at equilibrium, it does not specify concentrations have to be equal. The student must have obtained the information about a system at equilibrium where Q =K from the lecture notes. While the student had a good beginning to his/her reasoning, he/she did not fully understand the concept of chemical equilibrium and its characteristics.

In the above responses (Response 2 and 3), both student had the correct symbolic definition of a system at equilibrium, i.e, K = 1. While the symbolic definition is right, the reasoning was incorrect. K = 1 does not imply equal concentration, rather it means equal rates. There are two reasons why students confuse K = 1 to equal concentrations.

The first being, the preconception of *equilibrium* stems from the idea used in everyday life, where equilibrium means equality of two sides, stability and static in nature (Schafer, 1984). The second being, equilibrium constant is defined as the ratio of concentration of products to reactants. Hackling and Garnett (1985) reported that students held a simple arithmetic relationship between the concentration of reactants and products. The simple arithmetic relationship here is K = 1, i.e., the numerator and denominator has to be equal. Hence, concentration has to be equal.

Since only one student in the control group retained the common misconception on the post-test, only thematic analysis of student's common misconception towards item 3 is shown. The thematic analysis can be found it Table 21. Examining the codes listed in Table 21, it is evident that they either fell either held an arithmetical approach (i.e., K =1, K=Q, equilibrium means equal) or they were recalling information from the lecture notes without processing it.

	Theme 2 – Characteristics of Equilibrium				
	Control group				
	Question 3: At equilibrium, in terms of concentration? (N=15)				
Ν	Sub Themes	Codes	Student quotes		
	Theme 3(a)				
4	Concentration of reactants and products is equal because equilibrium constant K=1	K = Q hence equal, K = 1 hence concentration equal, Equilibrium means equal, Definition – information recall	<ul> <li>C4: "I choose, A because, because of, at equilibrium, they have to be equal, as from the notes, I got the idea K is equal to 1"</li> <li>C10: "I just went with A, Yeah the notes said a system is at equilibrium when equilibrium equal 1"</li> <li>C8: "I forgot what exactly my logic was. I choose A this time, I mean, the lecture notes suggested, K=1 implies equilibrium"</li> <li>C5: "Yeah it was the definition, well K = Q that's went you reach equilibrium"</li> </ul>		

Table 21: *Thematic analysis of common misconceptions held by students on the post-test towards item 3.* 

For item 5 75% of students in the control group and 20% of students in the experimental group retained the common misconception reported in the literature, i.e., concentration of NO and NOCl are equal. While comparing the pre-test and post-test data for the common misconception held by participants for item 5, it is evident 50% of students in the control group held the misconception and 40% of students in the experimental group held the common misconception. While the percentage of students holding the common misconception for item 5 in the experimental group went down, the percentage of students holding a similar misconception in the control group went up. It is worthwhile to examine the transcribed response from students in both groups.

In the first scenario, the student's pre and post-test response from the experimental group will be compared. The purpose for including the pre-interview responses is the post- interview response does not contain the actual analogical model conceived by the student. While the student has given the analogical model, the student misinterpreted the meaning behind the simulation.

# Experimental group

### Incorrect answer with incorrect reasoning

### Pre-test

### **R**: So for #5, you are saying equilibrium shifts to right? why did you pick (c)?

**P:** I kinda think of the mole mole ratio again, I could be entirely wrong, I cannot, I was think if you had 2 NO, I mean if you got 3 on the left side and 2 on the right side + heat, you kinda got this big slope, it just wants to bounce it out, its basically spilling all on the right side, that's why I told myself it should shift to the right. Okay so if its at equilibrium, it kinda wants to shift to the right, so they can be both the same.

Item 5 was conceived as an alternative to item 3. In other words, item 3 and 5 represent the same meaning. If a student had a conceptual understanding of item 3, then ideally they should be able to decide the correct answer choice for item 5. In the above response, it is evident the student had conceived an incorrect analogical model. The student's model of a slope suggest the reaction is viewed as happening in one direction. Hence, the student suggest there will be more products when the reaction goes to completion. The post-test response illustrates

### Experimental group

### Incorrect answer with incorrect reasoning

### Post-test

In the post-qualitative interview response below, while the student has given the incorrect analogical model of a slope, the student did not demonstrate conceptual understanding. The reason being the student had chosen the correct answer for item 3 but an incorrect answer or item 5. As pointed out in the previous paragraph, items 3 and 5 carry the same meaning. The student started to develop doubts whether he/she answered item 3 correctly. In the end, the student decided to go in favor of the reasoning for item 5 over item 3.

*R:* For #5, you still decide to stay with *C*, sometimes staying with the answer is a good thing, why did you decide to stay with *C*?

*P*: *I* have been questioning A and B also, and I know, its like, since, NO and NOCl do exist in 2 to 2 ratio, I think they are trying to be equal, but they never will be, its like close but not there, I could have chosen B, but couldn't have chosen it.

*P: I think C because [long pause]* 

*R:* The reason I ask is, for # 3 you choose concentration of reactants and products constant over time, but for #5, you suggest they fluctuate why is that? Wouldn't that be contradicting?

P: I'm gonna say now, No, Yeah it definitely is contradicting.

*R*: Why did you change your opinion between # 3 and #5? Why you thought differently? You agree with 3 or 5 more? Which statement agree with the most?

*P: It's probably going to be #3?* 

*P: I was thinking the numbers themselves are different in the new equilibrium, so I thought K has to be higher, since NOCl has gone up, I thought it would shift towards right.* 

*P*: *I* think that's what I was thinking

The following transcribed responses were obtained from paticipants in the control

group. Three responses are shown below. As pointed out earlier in the previous

paragraph, the percentage of students holding the common misconception, i.e.,

concentration of NO and NOCl will be equal because they exist in a 2:2 to stoichiometry

has increased between the pre and post-qualitative phase.

# Control group

# Incorrect answer with incorrect reasoning

**R**: So what was your reasoning behind your choice for #5? I mean what made you pick the particular choice?

# Response1

*P:* I picked choice B for #5 because, both NO and NOCl got coefficients of 2, so when equilibrium is attained, they should both be in equal amounts.

# Response 2

**P:** It says equilibrium, and when I saw 2 to 2, since its equal amounts, I figured that's sufficient information, so I decide to go with B

### Response 3

*P:* I choose *B*, honestly I was kinda not sure on this one, but I remember from the ICE table, you do -2x and +2x, so I kind felt that made sense.

In all three resposnes shown above it is evident that either a mathematical or algorithmic approach was seen. In particular response 3. The concept of ICE table is familiar among students who have learned the concept of chemical equilibrium. ICE stands for initial concentration, change in concentration and equilibrium concentration. The student has taken the right approach by setting up an ICE table. But the issue bein, the problem is qualitative in nature, hence it would not be possible to determine numerical value of equilibrium concentrations. I noticed a discountinity between applying the knowledge acqurired from a quanitative situation in to a qualitative situation. Another aspect that has been visible throughout the study has been incorrect application of the principle of stoichioimetry (Response 1 and 2).

Finally, the item that will be discussed under the common misconceptions category will be item 8. 42% of students in the control group and 40% of students in the experimental group held the common misconception, i.e., equilibrium constant K will be greater when equilibrium re-established following a decrease in the volume of the system. In contrast, 40% of students in the control group and 33% of students in the experimental group held this misconception. It would be worthwhile to discuss participant reasoning behind item 8.

The simulation on the two body connected to a pulley was developed to help students understand the concept of equilibrium constant better. Many students hold the common misconception that when reactant is added to a system at equilibrium,

equilibrium will shift to the right and make products. In other words, they tend to have a unidirectional view of a system that is occuring in both directions. The reasoning suggested by Cheung (2004) supports the view that incorrect application of LCP can lead to incorrect answers. Cheung (2009) further emphasized that chemistry teacher educators, textbook writers, school teachers must be educated on the inadequacy of LCP. The reason being, classroom instruction pertaining chemical equilibrium involving LCP, often expect students to predict the direction of equilibrium shift. Majority of textbooks even provide a table listing the direction of equilibrium shift using LCP, when a system at equilibrium is altered. Instruction does not focus on what happens to the system when it re-attains equilibrium. Rather the instruction focuses on direction of equilibrium shift. Providing students with a table that lists equilibrium shifts under different conditions, incorporates an algorithmic view in the minds of students.

# Experimental group

### Incorrect answer with incorrect reasoning

### Response 1

*R*: *So*, *you went* (*a*) *to b for #8*.

*P:* the pre-test I totally guessed, let me be honest. When you add NO, you gonna end with more products

**R**: Was the pulley experiment helpful at all

**P:** So it should be (a) then, dang

**P**: I got it wrong did I?

### Response 2

#### *R*: Okay, #8, what was your reasoning behind #8?

*P:* For #8, I was thinking, trying to remember prior knowledge, about what we learned in class, we learned a few tricks, like, more products added, the K go this way, whatever and took a guess, if you add more reactants, it shifts to the products

The discussion in the succeeding paragraphs discussion will describe misconceptions not reflected in the research literature (Canpolat et al, 2006; Hackling & Garnett, 1985; Hameed et al, 1993) but held participants in the control and experimental group (Table 22). In particular discussion will be about item 11 and 6. Item 6 is a special case because it showed the least performance gain among participants in the experimental group. 42% of students in the control group and 47% of students in the experimental group held the additional misconception, i.e., at equilibrium, K is less than 1, because total moles of products is less. Item 6 conveys the same meaning as item 4 but at a more foundational level. In other words, if a system as attained chemical equilibrium, rate of the forward and reverse reactions will be equal. It was quite surprising that how higher percentage of students answered item 4 correctly post intervention with the simulation could not answer item 6 correctly. One aspect that was evident from student response was, they used the simulation to answer item 4, whereas for item 6, they focused exclusively on the chemical equation and did not consider the purpose of the simulation. Another aspect that was evident from the simulation was, if they considered the simulation then they literally counted the number of molecules on the screen and failed to consider the graphical information presented.

Table 22: Frequency analysis of additional misconceptions held by students in the control (C) and experimental (E) group on the post-test data. (NA = not applicable)

Category	Misconception %(C)	Misconception %(C)
Approaching equilibrium	(N=12)	(N=12)
Forward and reverse reaction increase at the same	33	0
rate	33	0
Concentration of reactants and products are equal	17	0
Concentration of reactants 3 times more than	17	20
concentration of products		
Concentration of reactants and products is	33	7
constant because K<1		
Characterisitics of equilibrium		
Concentration of products is greater, because	17	0
K>1		
Because Cl2 is a limiting reagent, there will be no	17	0
Cl2 left		
Equilibrium constant		
At equilibrium, K is less than 1, because total	42	47
moles of products is less		
At equilibrium, $K = 1$ , because concentration of	25	7
reactants and products are equal		
Changing equilibrium conditions		
At equilibrium, when concentration of NO is	17	20
increased, initially, rate of forward reaction will		
not change, because volume is kept constant		
When volume is decreased to a system at	8	20
equilibrium, initially, rate of reverse reaction		
decrease		
When volume is decreased to a system at	58	7
equilibrium, when equilibrium is re-established		
rate of reverse reaction increase		
When volume is decreased to a system at	83	13
equilibrium, when equilibrium is re-established,		
concentration of NO Cl2 will be lesser and NOCl		
will be greater than the initial equilibrium		

It is evident from the response below while the student had thought of choosing

option d, decide to opt out against it because equilbrium constant cannot equal to rates.

This assumption is partly because students who learn equilibrium learn equilibrium constant has a function of concentration. Ideally, equilibrium constant should be expressed as a function of rate of a reaction

## Experimental group

#### Incorrect answer with incorrect reasoning

*R*: So, its very interesting, on #6, you decide to go with a, and then but this time you decide to go with none of the above

*P:* I thought of the lab we just did, I remember like finding the equilibrium constant, and then I realized, each reaction has its own K, its not necessarily equal to K, so any of these can be right.

**R**: The reason I picked 6 is, because for 3 you choose C, now if you had chosen a for 6, wouldn't that be contradicting? Cuz constant does not mean equal to one.

*P:* I thought about d, its rate of the reaction, I wasn't sure if it was rate of formation, I thought K had its own specific value.

**R**: Well you have a good point, cuz students are not really told, what K = 1 really implies

As pointed out above the reason why students carry the misconception with respect to equilibriumc constant, i.e., equilibrium constant is expressed as a function of concentrations. In the response shown below from a student in the control group it is evident that the student was able to recall information pertaining to equilibriu constant, yet guessed to determine the answer choice.

### Control group

#### Incorrect answer with incorrect reasoning

**R**: Okay moving on to #6, so what was your reasoning behind #6?

*P:* I kinda forgot what K was, a little bit, I do remember it was products over reactants, and I knew that it would be NOCl squared over NO squared and Cl2. I kind guessed it to be less than 1, I just wasn't sure there either. I guessed products will be less than reactants.

## **R**: Very good, very good

For item 11, 83% of students in the control group and 13% students in the experimental group held the misconception, i.e., when volume is decreased to a system at equilibrium, when equilibrium is re-established, concentration of NO Cl2 will be lesser and NOCl will be greater than the initial equilibrium. Hackling and Garnett (1984) suggested, students who held this misconception do not fully understand the relationship between consumption of reactants and formation of products in a chemical reaction. The reasoning suggested by Cheung (2004) supports the view that incorrect application of LCP can lead to incorrect answers. Berquist (1989) reported that students often selected multiple choice answer on an examination dealing with chemical equilibrium without a corresponding level of understanding for the underlying concepts. Transcribed responses from students in control and experimental group towards item 11 is shown below. The first set of responses were from participants in the experimental group.

It is evident from the responses that students generally decide to use the algorithmic approach in solving the problem. It is a common practice in a chemistry coursework for students to use Le Chatelier's principle (LCP) to solve this problem. Students are usually taught how to predict the equilibrium shift when a specific change is made to a system at equilibrium. The prediction process is usually a shortcut method that allow students to solve problems pertaining to LCP on a test. The prediction process

usually taught in a coursework does not actually allow students to conceptually understand what happens to each species in a reaction attaining chemical equilibrium at the system level. For instance, while a decrease in volume increase the partial pressure of the system, a decrease in volume also increase the concentration of all species involved in the system instantaneously. The reason being molar concentration is number of moles over the total volume of the system. However none of the three responses shown below incorporates the idea of volume in the context of molar concentration.

# Experimental group

### Incorrect answer with incorrect reasoning

**R**: So #11, you decide to go with F, why you did go with a, d & e

*P:* I know there is this rule, which says decreasing volume means increase in pressure, favors the side with more or less moles, I don't know which one, I guessed the low moles sides, so NO and Cl will be less and NOCl will be greater.

### Control group

# Incorrect answer with incorrect reasoning

### Response 1

**R**: so for #11, you decide to go with F than G. why is that?

*P*: Well again, I made that mistake of reading it as NO, so this time around I went with decreasing volume, so if you decrease volume, reaction will move to the side with less moles, so there will be less NO, Cl2 and more NOCl. F made the most sense

## Response 2

**R**: So what was your reasoning behind #11?

*P*: Well if you decrease the volume, you go towards the side with less amount of gas, and that was on the right side. So equilibrium will shift towards right, and I selected choices that fitted the logic. That's how I ended up with a, d & e

In the succeding paragraphs discussion will be presented about correct responses held by participants in both groups. The responses will be compared for selected items to establish the effectiveness of the intervention and reasoning variation between participants in both groups. Frequency analysis of student holding correct response on the post-test is shown in Table 23.

For item 1, 93% of participants in the experimental group and 17% of participants held correct respose for item 1, i.e., rate of the forward reaction decrease as the reaction gets going. In contrast, for item 1 33% of participants in the experimental group and 25% of participants in the control grou held correct responses. It is evident from the percentage comparison between the pre and post-test, percentage of students who held correct responses has gone up significantly. Transcribed responses shown below compare reasoning between participants in both groups for item 1. Only representative student responses are shown. Responses (1 and 2) from participants in the experimental group suggest not only they chose the correct answer but also held a valid scientific reasoning. It is be to noted, the responses came from students who had incorrect respose and incorrect reasoning for item 1. In contrast while the paricipant in the control group had correct answer, the reasoning was incorrect. The participant suggested, rate of the forward reaction decreased because you have less products. While there is less products to start with decrease in forward rate equates to a decrase in reactant concentration. The second paricipant who's response is not shown here also chose a correct answer but could not provide a valid scientific reasoning.

Table 23: Frequency analysis of correct responses held by students in the control (C) and experimental (E) group on the post-test data. (NA = not applicable)

Item	Category	Correct	Correct
		%	%
		(C)	(E)
		(N=12)	(N=15)
	Approaching equilibrium		
1	Rate of forward reaction decrease as the reaction gets going	17	93
2	None of the above	25	67
	Characteristics of equilibrium		
3	Concentration of reactants and products constant over time	50	93
4	Forward and reverse reactions continue to occur, rates of	42	100
	forward and reverse reactions are equal and rates are		
	constant over time		
5	None of the above	8	67
	Equilibrium constant		
6	Equilibrium constant $K = 1$ , rates of forward and reverse	25	20
	reactions are equal		
8	After addition of NO to a system at equilibrium and when	33	53
	equilibrium is re-established, equilibrium constant K is the		
	same as before		
	Changing equilibrium conditions		
7	After addition of NO initially, rate of forward reaction will	33	47
	instantenously increase		
9	When volume is decreased to a system at equilibrium, initially,	0	13
	rate of forward and reverse reaction increase	-	
10	When volume is decreased to a system at equilibrium, when	0	87
	equilibrium is re-established, rate of forward and reverse reactions		
11	are equal and greater than initial equilibrium	17	60
11	When volume is decreased to a system at equilibrium, when equilibrium is re-established concentration of NO, Cl2 and NOCl	1/	60
	will be greater than the initial equilibrium		
	win de Steater man the mittar equinoritam		1

# Experimental group

Correct answer and correct reasoning

# Response 1

*R*: *Okay for #1, on your pre-test you decide to go with (e), and on your post-test you decide to go with (c), why is that?* 

*P:* Cuz, when I looked the simulations in the program, it showed, like, the forward reaction cuz, there is a lot, and there is none on the reverse, which makes sense, because, the reactants there's something compared to products, so there's going to be a lot of forward reaction, and over time it will slowly decrease as the products increase, it makes sense,

**R**: So when we say the rate of the forward reaction decreases what are we referring to?

*P*: We are referring to reactants, that is giving it away, meaning eaten up, to make products

Response 2

*R*: Okay, we'll start with #1, on the pre you had e, this time around you have c, why did you pick c this time around?

*P*: Well, cuz, on the program it showed, the rate of the forward reaction decreases as it gets going.

*R*: So when we say, rate of the forward reaction decreases, what are we really referring to? You can explain it to me in terms of reactants and products

*P*: *I* guess how many the molarity or the concentration over time.

**R**: What happens to the concentration of reactants and products?

**P:** Ummm, it's going down right?

Control group

Correct answer and incorrect reasoning

R: Okay, on your pre-test for #1, you had d, but this you have c, why is that?

P: Due to the fact, its approaching and not at equilibrium, that's why I decide to change my answer

R: so rate is decreasing?

P: Yes

R: what we mean by decrease in rate?

P: cuz you have less products, so rate decreases

For item 3, 93% participants in the experimental group and 50% of participants in the control group held correct response. In contrast on the pre-test, for item 3 60% of participants in the experimental group and 42% of participants in the control group held correct responses. While there is a marginal increase in the percentage of participants with correct response in the control group, percentage of students in the experimental group who held correct responses has gone up significicantly. Only representative student responses that were comprehensive (i.e., there was enough conversation between the researcher and the participant over the item) are shown below.

While participants from both group held correct response, participants from the experimental group not only had a correct response, but a valid scientific reasoning such as system attains equilibrium when the rate of forward and reverse reaction is equal. A higher percentage of students in the experimental group on the pre-test held the opinion, a system is at equilibrium when concentration of reactants and products are equal. The student also further add how the simulation allowed to visualize the process through which a system attains equilibrium.

### Experimental group

### Correct answer with correct reasoning

*R*: *Okay for #3, you may have changed your answer, that does not mean it's right or wrong? For # 3 you choose (a), on your post-test you decide to go with (c), why is that?* 

*P:* I kinda realize, after seeing the graph, the reactants aren't going to be the same at equilibrium, so K very might well equal 1, not because products, I mean concentration of

products and reactants may not be the same, its just K expression is equal to 1, because its

**R**: So why do we say K equals 1. I mean, I really understood your logic, If in algebra we say, the ratio equals 1, what do we assume?

*P*: Well, if you assume, your ratio is 1, you have the same amount on one side and the same on the opposite side.

*R*: So if we say its constant as in (c), right, but we say equilibrium means K equals 1, what are we really refer to, these two cannot be equal, than how can K be equal to 1?

*P*: *I* would say the ratio of going from one end to the other is the same

*R*: so what is that ratio called? it's called by a different name.

**P:** May be rate?

Control group

Correct answer and incorrect reasoning

**R**: So now what was your reason behind choice for #3?

*P:* So, I remember, I remember, while learning, when you had equilibrium, I just remembered concentration of reactants and products are constant because, the rates were staying the same, so that's why I picked it

**R**: Very good, very good

For item 5, 93% participants in the experimental group and 50% of participants in the control group held correct response. In contrast, for item 3 60% of participants in the experimental group and 42% of participants in the control group held correct responses. There is a significant change in the percentage of students holding correct response in both groups. The percent went up in the experimenta group and went down in the control

group. It is to be noted, participants in the control group were allowed to use their lecture notes on chemical equilibrium prior to the post-test. Only representative student responses that were comprehensive are shown below. Comparing both responses it is evident, participant in the experimental group used a system's view to solve the question, while participant in the control group employed process of elimination to arrive at the answer. Closely examing the participant response from the experimental group, the student hold's a dynamic view of the system, i.e., making a change to one component of the system will affect other components of the system. A similar reasoning was not seen in the response from the participant in the control group. The participant in the experimental group also suggest how the visualization was helpful in understanding the dynamic nature of equilibrium.

# Experimental group

#### Correct answer with correct reasoning

*R*: *Okay* #5, you indicated a (b) on your pre-test, this time you decide to go with (d) why is that?

*P:* Again, because NO and NOCl exists in a 2 to 2 stoichiometry, there won't be equal amounts of NO and NOCl. I think the visual part of the thing, it was, it is, it really helped me to understand what the concentrations would be. Concentrations of NO, Cl2 and NOCl did not go to one thing, it were, it was, you know, NO was its one thing, Cl2 was its one thing

*R:* Okay, will it ever be the same? Under any circumstances would it ever be the same? Can we say that? If it's not equal, what makes it that way?

*P:* Because equilibrium is dynamic, when you change one thing, in this case if you change NO, you change two others, so I think that's probably why

#### Control group

### Correct answer with incorrect reasoning

**R**: Alright, so what was your choice behind #5?

*P:* Ummm, so they do have a 2 to 2 stoichiometry, I knew that at equilibrium, C wasn't going to be right, as it doesn't shift, I don't think Cl2 is going to be a limiting reagent, cuz its at equilibrium, I thought B sounded right, as we did ICE table, but couldn't get an answer cuz no numbers were given, so went with D.

For item 10, 87% participants in the experimental group and 0% of participants in the control group held correct response. In contrast, for item 10 20% of participants in the experimental group and 0% of participants in the control group held correct responses. There is a significant change in the percentage of students holding correct response in the experimental group, while there is no change in the contol group. Only representative student responses that were comprehensive are shown below. Comparing both responses it is evident, participant in the experimental group used a system's view to solve the question, while participant in the control group employed process of elimination to arrive at the answer. Only representative student responses that were comprehensive are shown below. Comparing both responses it is evident, participant in the experimental group used a system's view to solve the question, while the participant in the control group employed LCP to arrive at the answer. The response shown in the experimental group came from the same participant. The participant was able to move away from the idea of concentrations being equal to rates being equal post intervention. In addition, the participant was able to meaningfully integrate the effect of volume towards an increase in

the concentration of all species. In fact, it is the increase in concentration of all species leads to an increase in rate in the second equilibrium. Response from the participant in the control group concurs with the algorithmic view reported by Hackling and Garnett (1985) and Cheung (2009). Hackling and Garnett (1985) reported that students held a simple arithmetic relationship between the concentration of reactants and products. Cheung (2009) stated, instruction does not focus on what happens to the system when it re-attains equilibrium. Rather the instruction focuses on direction of equilibrium shift. Providing students with a table that lists equilibrium shifts under different conditions, incorporates an algorithmic view in the minds of students.

## Experimental group

### Correct answer with correct reasoning

**R**: For #10, you indicated (c) as your choice, this time you decide to go with (f), what was your reasoning behind the change?

*P:* Okay when new equilibrium is re-established after decreasing the volume, which means you increase the pressure, rates of forward and reverse reaction will be greater than before, so,

- **R**: Why do you think its greater?
- **P:** Rate = k\*times.
- **P**: I don't think that's right,

**R**: No go ahead and complete it, this is one way of writing it

- **R**: So how did we define rate earlier in our interview?
- **P:** We said concentration over time
- **R**: Why do you think rate is greater, what made rate greater?

*P:* more stress on reactants and products, to compensate, subsequent increase in NOCl, there is also going on in the reverse direction,

**R:** So what is increased in the ratio?

*P*: *The concentration of the products and the reactants?* 

**R**: Very good, good

Control group

# Incorrect answer with correct reasoning

*R*: So what was your reasoning behind #10?

*P:* Okay, even though you decrease volume, some of the stuff will moves to the right, but when equilibrium is established forward and reverse rates will be equal. I knew it right away. That's why I decide to go with choice f

For item 11, 60% participants in the experimental group and 0% of participants in the control group held correct response. In contrast, for item 11 27% of participants in the experimental group and 0% of participants in the control group held correct responses. There is a significant change in the percentage of students holding correct response in the experimental group, while there is no change in the control group. Only representative student responses that were comprehensive are shown below. Comparing participant responses from the experimental group to the participant response in the control group it is evident, participants in the experimental group used a system's view to solve the question, while the participant in the control group employed LCP to arrive at the answer. The responses shown in the experimental group came from the identical participants. Both participants were meaningfully able to integrate the change in volume to change in molar concentration.

# Experimental group

# Correct answer with correct reasoning

# Response 1

*R*: Alright for #11, you clearly had a change of answer, what was your reasoning behind your change of answer?

*P*: Well the simulation explained concentration well, well concentration is moles over liters, so if smaller volume, concentrations going to be higher for all, I mean reactants and products

# Response 2

*R*: *Okay, another question where you clearly changed your opinion is #11. Why is that, I mean what was your reasoning behind your change? You had (f) now you have (g)* 

*P:* The concentration graph when you decrease the volume was helpful. When you decrease the volume, you are increasing the concentration, of all of em, because its moles over volume,

# Control group

# Incorrect answer with correct reasoning

**R**: so for #11, you decide to go with F than G. why is that?

**P:** Well again, I made that mistake of reading it as NO, so this time around I went with decreasing volume, so if you decrease volume, reaction will move to the side with less moles, so there will be less NO, Cl2 and more NOCl. F made the most sense

### **ANCOVA ANALYSIS**

An ANCOVA analysis was conducted to the answer the overall research question and research hypothesis 1 of this study,

**Research question:** Is there is a statistically significant difference in the means between the control and the experimental group at posttest, after adjusting for pretest scores?

**Research hypothesis 1:** A mean difference in posttest scores will occur between the control and experimental group, after adjusting for the pretest scores.

### ANCOVA

A one-way analysis of covariance (ANCOVA) evaluates whether population means on the dependent variable are the same across levels of a factor, the independent variable, adjusting for differences on a covariate (i.e., whether the adjusted group means differ significantly from each other). The independent variable divides individuals into two or more groups, while the covariate and the dependent variable differentiate individuals on quantitative dimensions (Green & Salkind, 2003). The purpose behind conducting an ANCOVA is to compare the two group's (control and experimental) posttest scores after removing the effects of subject heterogeneity, or naturally occurring individual differences during the pretest.

### **ANCOVA** Assumptions

The following ANCOVA assumptions were tested and found tenable, before the ANCOVA was performed on the data obtained from the dissertation study.

**Assumption 1:** The dependent variable and the covariate variable should be measured on a continuous scale. The assumption was met, because the dependent variable (post-test scores) and the covariate (pre-test scores) were measured on a continuous scale.

**Assumption 2:** Independent variable should consist of at least two categorical groups. The independent variable consisted of control and experimental group (categorical). The experimental group received the intervention in the form of computer simulations.

**Assumption 3:** Independence of observations. There was no relationship between the observations within each group or across groups because participants in the control and experimental group met on separate occasions and participants could not share or discuss the material being learned during the experiment.

**Assumption 4:** The dependent variable is approximately normally distributed within each category of the independent variable. Shapiro-Wilk test of normality was performed and the p value was greater that .05 (experimental group = 0.232 and control group = .065) suggests, the data is approximately normally distributed within each condition. In addition, skewness and kurtosis data was used to establish normality. As reported in George and Mallery (2010), values for skewness and kurtosis between -2 and +2 are considered acceptable in order to suggest data represent an approximately normal univariate distribution. Skewness for experimental and control groups are respectively (-0.37 and 0.47) and kurtosis for experimental and control group respectively (1.73 and -0.33) fell under the skewness and kurtosis range for normality suggested in George and Mallery (2010). Assumption 5: Homogeneity of regression slopes (i.e., there is no interaction between the covariate and the independent variable). Interaction effect between the dependent categorical variable (group) and the covariate (pre-test scores) to establish homogeneity of regression slopes. Homogeneity of regression was tenable. F(3, 16) = 3.01, MSE = $65.21, p = .06, \eta_p^2 = .36.$ 

**Assumption 6:** Test of homogeneity of variance, the spread of scores within each condition (treatment and control) should be approximately similar. A Levene's test of equality of error variances was conducted to establish homogeneity of variance between the two conditions. If the Levene's test result is statistically significant, it means that the data do not show homogeneity of variance. If the Levene's test is not significant, then the assumption of homogeneity of variance is tenable. The p value was found to be .948. which, suggests that there is little evidence that the group variances are not equal and the condition of homogeneity of variance is tenable.

**Assumption 7:** The covariate is related to the dependent variable (post-test scores) at each level of the independent variable (group – control/experimental). The assumption was tested by creating a grouped scatter plot between the covariate, the dependent and the independent variable. The slopes for each group are plotted in the scatter plot of the data points with the covariate (pre-test scores) on the x axis and the dependent variable (post-test scores) on the y axis. The scattered plot indicated that the variability in the groups around the regression slopes is much reduced as compared to the variability around the mean, as indicated by two lines that run almost parallel to each other. The results from the grouped scatter plot suggest, the assumption that the covariate is related to the dependent variable at each level of the independent variable is reasonable.

#### Results

Results from a one-factor ANCOVA showed posttest scores were significantly higher for the experimental group ( $M_{\text{postadj.}} = 7.27 \ SD_{\text{post}} = 1.387$ ) relative to the control group ( $M_{\text{postadj.}} = 2.67, \ SD_{\text{post}} = 1.371$ ) after adjusting for pretest scores, F(1,24) =71.82,  $MSE = 1.497, p = 0.03, \eta_p^2 = 0.75, d = 3.33$ .

Cohen's d was converted to an attenuated effect size d\* using the procedure outlined in Thompson (2006). The adjusted (for pretest scores) group mean difference estimate without measure error correction for the posttest scores and the pretest scores was 4.2 with a Cohen's d = 3.04.

An alternate approach reported in Cho and Preacher (2015) was used to determine effect size. The adjusted (for pretest scores) group mean difference estimate with measurement error correction only for the posttest scores (but not with measurement error correction for the pretest scores) was 4.99 with a Cohen's d = 3.61. Finally, the adjusted (for pretest scores) group mean difference estimate with measurement error correction for both pretest and posttest scores was 4.23 with a Cohen's d = 3.07. From a quantitative perspective, these effect size indicate a strong relationship between the experimental intervention provided and students' conceptual understanding of chemical equilibrium concepts. That is, those students who received the experimental intervention had exceptionally higher In summary, the above section on the post quantiative/qualitative analysis provides evidence that participants in the experimental group were able to apply system principle while solving a question. In the next section (Chapter 5) summary of the findings from the research study along with implications recommendations for future research will be provided.

#### **Simulation Notes-Sheet**

The major purpose for incorporating the simulation notes into the study was to identify information students extracted from their interaction with the simulations. An assumption made in this case is that it is important, as it allows the researcher to determine whether students were able to transcribe the audio in their notes or is it more the visual component that they find beneficial or a combination of both. Representative snap shot of students writing is shown below. Student feedback obtained through the simulation notes sheet will be used to update future versions. In addition student feedback will be used in the context research questions discussion in the final chapter (Summary & Conclusions).

Figure 5 shows aspects of simulations that was appreciated by participants. The one aspect that was unanimously appreciated by all participants was the existence of graphical displays in the simulations.

Figure 5: Aspects of simulation appreciated by students

It is evident from Figure 6, the visual aspect of the simulation is dominating. Even examining writings displayed in the figure and even in ones that are not displayed in the collage, students unanimously agreed that they found the graphs helpful. In particular, simulation notes from participants suggest, they particularly understood the concept of rate more clearly through the three stages: a) when the system was approaching equilibrium, b) when the system has attained equilibrium and c) when a change has been made to a system that was at equilibrium. It is apparent from Table 32, percentage of students who answered items 1, 2, 4, 5, 7, 10 and 11 correctly between the pre and post-test increased. Items 1, 4, 7, 9 and 10 tested participants understanding of the concept of rate under three stages: a) when the system was approaching equilibrium, b) when the system has attained equilibrium and c) when a change has been made to a system that was at equilibrium. While not shown in Figure 6, participants demonstrated conceptual understanding of the concept of concentration. Participants who answered items pertaining to concentration change (item 2, 3 and 11) also had detailed notes and thorough description of their understanding behind the graphs relating concentration change as a function of time. All 15 students admitted during the post-qualitative interview that the graphs were very helpful towards understanding the various concepts. When inquired, if they did not find the particle view helpful? Most students did suggest, they did find it helpful, however the combination of audio cues and the graphs were very helpful.

Simulation 5 Notes " $\mathcal{D}$ ratio does not change $\mathcal{U} = \frac{\mathcal{P}}{\mathcal{A}}$ does not change	re eithr.	
"You are done with this experiments." good.	Simulation 7 Notes	<ul> <li>A timetering then but beging liken same increases created is still glitchy.</li> <li>I books like they non all snug fitted after decaase vehave.</li> <li>A concentrimities is biogra as notes can't freely nonce in boordar vehave, thus betrake technication.</li> </ul>
Simulation 3 Notes $*$ rote $[t]$ charts high because you, $(t)^{\pm}$ If bestically balances out have reactivelys and deceases (to form product) * decreases (as products one being found) * rate $(t)$ shorts nore (because there is none) * decreases (as products one being found) $*$ rate $(f)$ $[t]$ $rate (r) = \frac{1}{r} r* reactively [rate (r) = \frac{1}{r} [t]$	Pardants highly	decrease, NOCI increases. They never equal, then products. Remain constant around 40 seconds
Simulation 4 Notes * add more whight on d2, d2 will go to be as it kinds which to fit to be as it kinds which to fit as it kinds which to fit a	ist	Mar [NO] them previous eq., but goes to vact on the light
Simulation 4 Notes Al aquilibrium, the rate are the same the fortunard Martian Moreaner, then Must decrease once the forese reaction begins		more NOCI, NO, less Ciz or 29.

Figure 6: Content aspect learned by students through the simulations

#### **CHAPTER V. SUMMARY & CONCLUSIONS**

#### **Summary of Findings**

The purpose of this study was to evaluate the effectiveness of simulations in supporting post-secondary level students' conceptual understanding of chemical equilibrium at the particle level (microscopic). The conditional probability analysis indicated a recurring pattern i.e., a participant who correctly responded to an item (item 1) with in a category (for example, approaching equilibrium), had a higher probability of answering another item (item 2) correctly with in the category.

Results from a one-factor ANCOVA showed posttest scores were significantly higher for the experimental group ( $M_{postadj.} = 7.27 SD_{post} = 1.387$ ) relative to the control group ( $M_{postadj.} = 2.67, SD_{post} = 1.371$ ) after adjusting for pretest scores, F(1,24) =71.82,  $MSE = 1.497, p = 0.03, \eta_p^2 = 0.75, d = 3.33$ . Cohen's d was converted to an attenuated effect size d\* using the procedure outlined in Thompson (2006). The adjusted (for pretest scores) group mean difference estimate without measure error correction for the posttest scores and the pretest scores was 4.2 with a Cohen's d = 3.04. From a quantitative perspective, the larger effect sizes indicate a strong relationship between the experimental intervention provided and students' conceptual understanding of chemical equilibrium concepts. That is, those students who received the experimental intervention demonstrated significantly higher conceptual gains in understanding chemical equilibrium than students in the control group who were permitted to review their notes, but that did not have any additional intervention. It is important to note that several weeks before the study was conducted chemical equilibrium had been presented and tested on the mid-term exam of the general chemistry course in which both groups were enrolled. , Therefore, the understanding both groups held about chemical equilibrium was found to be similar based on the results of the pre-test.

The Kuder-Richardson 20 (K-R 20) analysis was performed to determine the reliability of the instrument. The K-R 20 was specifically used in reliability analysis because, K-R 20 is a special form of Cronbach's alpha that is used when the quantitative instrument contains dichotomous data (right or wrong responses) and when the response data does not represent a continuous scale or cannot be ranked in any particular order. The value of Cronbach's alpha for the post-test was acceptable ( $\alpha = 0.71$ ) falling with the range of acceptable values ranging between 0.7 to 0.95 (Devills, 2003; Nunnally, 1994). Comparing the pre and the post-test Cronbach's alpha, there is a sharp increase suggesting that there is more inter-relatedness between the items, and suggesting that perhaps the number of items is sufficient.

Instruments that have been used by researchers (i.e., Canpolat et al, 2006; Hackling & Garnett, 1985; Hameed et al, 1993) to identify student misconception towards chemical equilibrium for the reaction shown in Equation 1 has involved obtaining a true or false response or the test containing a limited number of choices – typically only three (i.e., increase, decrease or none). Such assessments provide a chance of 50% and 33 % , respectively, that a student could guess the correct answer choice without understanding the content.. Ozmen's (2008) two-tier instrument focuses on multiple chemical reactions. While a two tier instrument (Ozmen, 2008) might be helpful towards understanding student misconceptions towards multiple chemical reactions, for an intevention based study, an instrument focusing on a single reaction, yet addressing

multiple facets of chemical equilibrium is essential. It is to be noted, due to time constraints, chemical equilibrium misconceptions on topics centred around effect of catalyst, temperature and inert gas on a system at equilibrium was not addressed in the current study. Hence the instrument did not seek to understand students understanding towards those concepts.

#### Discussion

This section presents a discussion on the major findings that emerged from this study. The discussion is framed around the four research questions that guided the study. Percentages of responses from the experimental group and control group are presented in parentheses, where the first number correlates to the percentage of experimental group's responses, and the second number correlates to the percentages of control group's responses.

# **Research Question 1: What are students' conceptual understandings of chemical equilibrium before interacting with the simulations?**

Table 14 summarizes the frequency analysis of common misconceptions held by students in the experimental and control group. Common misconceptions refers to conceptual misunderstandings that have been identified by prior research (Wheeler & Kass, 1978; Hackling & Garnett, 1985; Banerjee, 1991; Huddle & Pillay, 1996; Voska & Heikkinen, 2000) on the topic of chemical equilibrium. While numerous studies have identified chemical equilibrium misconceptions held by students over the last 2 decades, specific studies that focused on student misconceptions towards the chemical reaction shown in Equation 1 listed in Table 14. Common misconceptions held by a higher

percentage of students in the control and experimental groups respectively, included: a) concentration of reactants and products at equilibrium are equal (item 3a, 33%, 27%) b) equilibrium constant K is greater for the specific chemical reaction when equilibrium is disturbed and re-established (8b, 40%, 33%), c) at equilibrium concentration NO and NOCl will be equal because they exist in a 2 to 2 stoichiometric ratio (5b, 50%, 40%), d) after addition of NO, rate of forward reaction increase and reverse reaction decrease (7e, 25%, 87%) and e) when volume of the system is decreased and equilibrium is re-established, rate of forward and reverse reactions will be same as that of the initial equilibrium (10d, 25%, 60%).

A major difference between the current study and the studies identified in Table () (Canpolat et al, 2006; Hackling & Garnett, 1985; Hameed et al, 1993) is, the current study employed a quantitative instrument with multiple distractors for each item. Additional misconceptions held by students in both groups during the pre-phase shown in in Table 15. Additional misconceptions are not merely wrong choices, but distractors carefully chosen from various research studies. For instance, the answer choice, "while a system is approaching equilibrium" only the rate of the reactions were explored in prior studies, the aspect of concentration while a system approaching equilibrium was omitted. Similarly, while research studies have identified student's misunderstanding and misapplication of Le Chatelier's principle, instruments have not quantified students' misconceptions, at least towards the chemical system shown in equation 1. For instance, a higher percentage of students in both groups held an algorithmic view towards solving item 11. Research studies (Cheung 2004, 2009; Hackling & Garnett, 1985; Hameed, Hackling & Garnett, 1994) have identified that students tend to apply Le Chatelier's

principle in a formulaic method, for this reason, the algorithmic view was created as a distractor in item 11. As expected, student responses confirmed the formulaic view reported in the literature. A higher percentage of students in both groups did not have a system's view and applied Le Chatelier's principle in a logical manner (Shafer, 1984; Berquist, 1989).

Representative interview responses shown below for item 11 illustrate how students in the experimental and control groups demonstrated a formulaic view reported in the research literature. More specifically, they held the view that equilibrium within a system occurs in one direction, rather than in both directions (Hackling & Garnett, 1985; Hameed, Hackling & Garnett, 1994).

In the representative responses shown below it is evident that students not only hold an incorrect view about stoichiometry, but also failed to integrate the effect of volume. If the volume of a system is deceased, then molar concentration (moles over volume) should increase for all species within the system. Such an explanation was not found in student responses. Instead, student's response reflect a see saw model view, i.e., when two people of equal weight sat on a see saw and when additional weight is added to one side, then the side with more weight goes down and the side with less weight goes up.

#### Experimental group

Student: "So you go to the side with the least amount of stress, so we go to right, going to (d), we have the concentration of Cl2 will be less than first, and the concentration of NOCl would have to increase as in (e)"

#### Control group

Student: "Decrease volume means increase pressure, 3 moles on the reactant side and 2 moles on the product side, it's gonna shift to the side with less moles, and I know that the reaction is going to shift to the right, to decrease the pressure, the NO and Cl2 would decrease and NOCl would increase"

# **Research Question 2: What key characteristics of students' mental model regarding chemical equilibrium concepts can be extracted from the qualitative data before viewing simulations?**

According to Greca and Moreira (2000), mental model is defined as personal, internal representations used by learners to explain and make predictions about the world surrounding them. Alternatively Coll and Treagust (2003) assert that mental representations that include mental models are the personal representations of a concept or entity that resides in the mind of the knower. They presented the view that it is not easy to understand mental models, as students often describe ideas they may not have understood properly.

According to Bodner (1986), individuals learn as a result of an active process in which individuals construct their own knowledge through interaction of the physical environment with their existing experiences. Thus, the initial mental models that students bring to a learning environment are different from each other and therefore, different learners construct identical meanings differently.

In addition, Chi (1994) notes that conceptual change occurs when a concept is reassigned from one category to another. She asserts that all entities belong to one of the three ontological categories; a) entities, b) process and c) mental States. According to Chi's conceptual change model, a concept such as chemical equilibrium contains constraint based features like randomness, simultaneous, uniform activities. A constraint

based interaction (CBI) provides no information about its time course, because it has no time element.

The constraint based features might prevent students from deeply understanding the concept of chemical equilibrium. Concepts associated with chemical equilibrium such as rate of a reaction, molar concentration, equilibrium constant are also part of the CBI category. CBI and events are sub-categories of the event ontological category. Examples of events include; a reaction is dynamic or static, a reaction is happening in one direction, a reaction is happening in both direction. If a student add or delete concepts with in an event or CBI category, a basic conceptual change is achieved. If a student's thought process switches from an event sub tree to a CBI sub tree or a switch from a matter to process category then a radical conceptual change is achieved.

A coding taxonomy was developed to explain how student's conceptual model shifts between ontological categories. The taxonomy is shown in Figure 7.

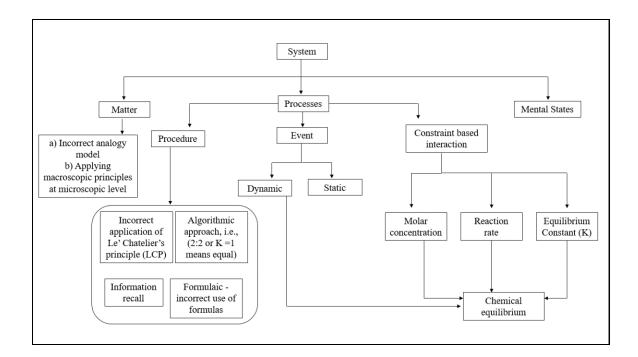


Figure 7: Coding taxonomy developed to explain student's conceptual shift between ontological categories.

As chemical equilibrium is a complex system, the term system was chosen as the foundational component of the hierarchical tree. Ontological categories (matter, processes and mental states) proposed by Chi et al (1994) were chosen as the three sub branches of the system component. Sources of alternate misconceptions identified in the literature were grouped under a specific ontological category or under a sub branch of an ontological category.

For example, Gussarsky and Gorodetsky (1990) reported that applying macroscopic qualities to the microscopic level leads to alternate conceptions in understanding of chemical equilibrium. The use of models (analogic models), which are known to possess limitations, is one way of differentiating scientists and experts from students and novices. Experts have a greater level of experience with phenomena and models, as well as the culture and norms of chemistry. Experts have greater ability to visualize abstract concepts, whereas "novices usually have incomplete or inaccurate models, whereas those held by experts includes macroscopic data from the physical world and formal abstract constructs of the phenomena" (Williamson & Abraham, 1995, p. 522). Grosslight, Unger, Jay and Smith (1991) claim that novices tend to think of models in concrete terms, meaning that novices think of models as scale models of reality – the ball or sphere used in teaching really is exactly like an atom – apart from its size. Research indicates that experts recognize the purpose of models, that is, that models are intended to serve the user and frequently require modification as new experimental data are revealed. Students fail to understand that models, no matter how successful and realistic appearing, are not copies of reality.

Similarly Nakleh and Krajcik (1994) suggested that students construct most of the understanding of chemistry from a macroscopic perspective and fail to relate the macroscopic representations to symbolic and microscopic representations. Sudents' qualitative reasoning in both control and experimental groups, exhibited matter level understanding, i.e., either they had developed incorrect analogical model or have applied analogical models, then the reasoning would be grouped under the matter category.

Chemistry instruction at the secondary or post-secondary levels typically focus on two of three levels, predominantly the macroscopic and the symbolic levels. Instruction at these two levels does not automatically render comprehension of the microscopic level among students, nor does it allow students to transition between levels like chemists do (Nurrenbern & Pickering, 1987; Nakhleh 1993). Results of the these studies suggest that students with varying academic levels perform better on chemistry

questions that are algorithmic/mathematical in nature, even towards questions that involve the sub microscopic level. Nurrenbern and Pickering (1985) demonstrated through their research study that many students were able to give correct numerical answers without applying content knowledge in solving chemistry problems. Gabel (1981), found that students were able to solve chemistry problems by application of algorithms that was not dependent on content knowledge requirement. According to Herron (1996), "algorithms are carefully developed procedures for getting right answers to exercises and routine tasks within problems with a minimum effort" (p. 64). Anamuah-Mensah (1986) suggested that instructors and teachers found it easier to teach chemistry problems through algorithms and formulas, thus ignoring the key aspect of conceptual knowledge.

In their review of research on chemistry problem solving, Gabel and Bunce (1991) found that students used what was referred to as a Rolodex approach, whereby they searched through memorized formulas until finding one where the units in the data matched the units in the problem. Solving chemistry problems in this manner focuses students' attention on symbolic representations rather than developing a conceptual understanding that integrates symbolic and microscopic representations.

Pushkin (1998) listed four reasons to describe the disparity between conceptual understanding and algorithmic approach towards solving chemistry problems. They are a) students enrolled in general chemistry tend to follow a set of procedures and rules in solving problems, b) students display dualistic behavior – either act as repositories of knowledge, accepting information their instructors tell them without questioning it or accept their instructors perspective only under testing conditions, c) novice learners are

subject to science curriculum and pedagogy that discourage critical and conceptual thinking and finally d) instructors who teach such classes also place more value on algorithmic learning than on conceptual learning, leaving the learners with the impression that science is "math in disguise" (p. 809). This aspect of algorithmic application of concepts towards solving chemical equilibrium problems will be one of the ideas explored in the study. Cheung (2009, 2004) have suggested while Le Chatelier's principle (LCP) is deceptively easy to apply to solve chemical equilibrium problems, LCP is inadequate and can result in incorrect predictions about the effect of changes in concentration, volume, pressure or temperature on a chemical system at equilibrium. They concluded LCP is not a pre-requisite towards a deeper conceptual understanding of chemical equilibrium. Cheung (2009, 2004) suggested while teaching chemical equilibrium in classrooms teachers must not rely exclusively on LCP and should promote real learning by leaning towards the use of equilibrium law, concept of reaction quotient, and the simplified version of Van't Hoff equations.

Hence, the four common sources of alternate conceptions (information recall, algorithmic application, incorrect application of LCP and formulaic application of logic) were chosen to be part of the procedural ontological category. Qualitative interview during the pre-test for the experimental group were analyzed to determine if students held the above common sources of alternate conceptions. If a student had answered an item correctly but had used any of the four sources, then the number of students who held the incorrect model will appear in bold in the coding taxonomy shown in Figure 8, while the student had answered an item incorrectly and used any of the four sources, then the number of students will appear in italics in the coding taxonomy shown in Figure 8.

The preconception of *equilibrium* stems from the idea used in everyday life, where equilibrium means equality of two sides, stability and static in nature (Schafer, 1984). While systems that reach chemical equilibrium may appear macroscopically stable and static, microscopically the system is dynamic not only because of molecular movement but also because the process of bond breakage and creation goes on. Equilibrium constant is defined as the ratio of concentration of products to reactants. Hackling and Garnett (1985) reported that students held a simple arithmetic relationship between the concentration of reactants and products. The simple arithmetic relationship here is K = 1, i.e., the numerator and denominator has to be equal. Hence, concentration has to be equal.

According to Ben-Zvi et al (1987) and Krajcik (1991), alternate conceptions about chemical concepts arise from a) representing chemical concepts only at the macroscopic level rather than in combination with microscopic and symbolic level b) comprehending chemical concepts at the macroscopic level through surface features and c) interpreting chemical reactions as a static processes. Ben-Zvi et al (1987) reported that despite substantial instruction, students in the study viewed formulas were merely abbreviations for names rather than a composition or a structure. Hence, dynamic and static views about chemical equilibrium were included under the event ontological category. Whether students hold a static or dynamic view was examined through analysis of the prequalitative interview.

Concepts associated with chemical equilibrium such as rate of a reaction, molar concentration, equilibrium constant are also part of the CBI category. CBI and events are sub-categories of the event ontological category.

Molar concentration refers to the ratio of total moles of solute to the total volume of the system. If for instance a student had a correct answer choice on an item pertaining to concentration, but the reasoning did not contain a scientific explanation of molar concentration involving terms such as moles of solute or volume of a system, it would be deemed that the student do not have a conceptual understanding of the CBI category molar concentration. Students who fell under this view of correct answer but insufficient or incorrect explanation indicated by dotted arrow in the coding taxonomy shown in Figure 8. # of students who held this model will be shown in parenthesis along the arrow. In contrast, if a student held a correct answer a correct scientific reasoning on items pertaining to concentration, then such a mental model indicated by a bold arrow in the coding taxonomy shown in Figure 8. # of students who held this model will be shown in parenthesis along the arrow. Items that represent concentration aspect of chemical equilibrium will also be shown.

According to Hackling and Garnett (1985), students generally had a qualitative understanding of the way in which the concentration of reactants and products changed as the reaction approached equilibrium. The misconception may result from students' prior experience with chemical reactions which do in fact show an increase in rate as the reaction takes place. For example when a piece of magnesium (Mg) ribbon is placed in dilute acid, rapid evolution of hydrogen gas results. In these reactions, there are special factors that govern the increase in rate of a forward reaction. It is likely, students do not develop complete understanding of these special factors, but instead develop the misconception that the rate of a chemical reaction increases as the reaction proceed towards equilibrium. Because students have developed the misconception, rate of a

reaction in the forward reaction increases, they believe the opposite is true, i.e., rate of reverse reaction decreases. This misconception is further reinforced by misapplication of Le Chatelier's principle. Because classroom instruction continue to reinforce the idea, when the volume of a system is reduced the reaction would shift to the side with least moles (LCP), students associate the equilibrium shift with rate of a reaction.

Students who held such a mental model reported by Hackling and Garnett (1985) indicated by a dotted arrow in the coding taxonomy shown in Figure 8. *# of students who held this model* will be shown in parenthesis along the arrow. Alternatively, if students held scientifically acceptable conception for rate related concept. Student mental models will be indicated by a bold arrow as shown in Figure 8. *# of students who held either the alternate or correct conception* will be shown in parenthesis along with the items towards which they had a specific conception.

Bilgin (2006) suggested students memorize the rules they learn and then try to apply it without understanding, fixating on the pervasive set of reasoning rule-rote recalling algorithm. The development of this algorithmic misconception can be attributed to considerable emphasis placed on reaction stoichiometry in introductory topics Hackling and Garnett (1985); Hameed et al (1994). Hackling and Garnett and Hameed et al reported that students' lack of approaching the reaction from a system's perspective could be due to their lack of understanding of the way in which numbers of moles of reactants being consumed and products being formed in a chemical reaction are related. Cheung (2009) emphasized that instruction does not focus on what happens to the system when it re-attains equilibrium. Rather the instruction focuses on direction of equilibrium

shift. Providing students with a table that lists equilibrium shifts under different conditions, reinforces students applying an algorithmic view.

A combination of incorrect understanding of stoichiometry and algorithmic approach contribute towards students' alternate conception with the concept of equilibrium constant. Students who held alternate conception towards equilibrium constant indicated by a dotted arrow in the coding taxonomy shown in Figure 8. # of students who held this model will be shown in parenthesis along the arrow. Students who held scientifically acceptable conception for rate related concept. Student mental models will be indicated by a bold arrow as shown in Figure 8. # of students who held correct conception will be shown in parenthesis along with the items towards which they had a specific conception.

Conceptual understanding of chemical equilibrium require students to have a dynamic view of the system and be able to integrate constraint based interaction such as molar concentration, rate of the reaction and equilibrium constant in a coherent fashion. Such an interaction can be seen in coding taxonomy shown in Figure 8. Arrows from dynamic system, constrain based interactions (molar concentration, rate of the reaction and equilibrium constant) lead to the concept of chemical equilibrium.

Mental states were not the focus of the study and hence was not studied. Therefore a discussion on defining and applying the mental states ontological category is beyond the scope of the current study.

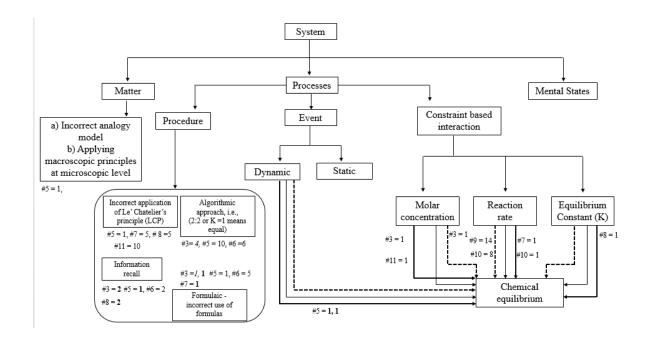


Figure 8: Coding taxonomy demonstrating mental model held by student's in the experimental group during the pre-intervention phase.

It is important to note that time was a major limiting factor in the study. This includes the time it took to recruit students to meet the necessary sample size for both the pilot and the research study, and the time a participant was willing to invest towards the study. Most participants spent about 90-120 minutes of their time to complete their portion of the study. If given more time to interact with each participant, greater detail from interviews might have been collected to richly portray participants' complex understandings of chemical equilibrium, and characterize potential changes in the experimental group's mental models after interacting with the simulation intervention. As it was, the detail collected from participant interviews provided sufficient evidence to illustrate key scientific understandings developed through interacting with after students completed the simulation intervention.

The most common of all chemical equilibrium misconception reported in the literature is the fact, students carry the notion that at equilibrium, concentration of reactants and products are equal (item 3 and 5). Items 3 and 5 are part of the larger theme, characteristics of chemical equilibrium. The preconception of *equilibrium* stems from the idea used in everyday life, where equilibrium means equality of two sides, stability and static in nature (Schafer, 1984). While systems that reach chemical equilibrium may appear macroscopically stable and static, microscopically the system is dynamic not only because of molecular movement but also because the process of bond breakage and creation goes on. Gussarsky and Gorodetsky (1990) explained applying macroscopic qualities to the microscopic level leads to misconception towards understanding of chemical equilibrium. Hackling and Garnett (1985) reported that students held a simple arithmetic relationship between the concentration of reactants and products. Berquist (1989) reported that students often selected multiple choice answer on an examination dealing with chemical equilibrium without a corresponding level of understanding for the underlying concepts.

To illustrate the functionality of the coding taxonomy only representative item and item responses are discussed. Key words are underlined to illustrate why a student's mental model fell under a specific ontological category.

Examining Figure 8 for item 3, it is evident that only 1 out of the 15 students in the experimental group held a scientifically acceptable view of chemical equilibrium. The transcribed interview response shown below demonstrates how the student held a scientifically acceptable view of chemical equilibrium. The student offers multiple view points while answering the question. The underlined words in the response below suggest

that the student justified why concentrations are constant over time at equilibrium, i.e., rate of the forward and reverse reactions are equal. The student was able to relate two CBI categories while answering the question.

**R**: So same with #3, why did you go with (c) why is that?

*P:* Well, ummm, concentration of reactants and products is <u>constant over time</u>, Ummm, equilibrium just means that, both <u>forward and reverse reactions are happening at the</u> <u>same rate</u>. So, the concentrations don't change otherwise manipulated, if left alone it will stay the same at equilibrium

In contrast, while two more students answered item 3 correctly, the responses do not have the same characteristics held by the student above. The underlined words suggest the student was merely recalling the definition of chemical equilibrium. Transcribed student response is shown below. The response also illustrates, the student was unable to explain the reasoning why concentration of reactants and products are constant at equilibrium.

**R**: So why did you decide to go with c for #3?

*P:* Ummm, this one was quite obvious, <u>I learned in lecture</u>, that equilibrium concentration is constant, cuz K = 1

**R**: Okay why you think its constant

**P:** Like I said, <u>cuz K = 1 its equilibrium and hence it constant</u>

Moderately higher percentage of students held an algorithmic view (procedural category) while solving item 3. Underlined words in student responses below illustrates the algorithmic view held by students.

Student 1

**R**: Okay for #3, This is the reaction has its shown here, you choice (a) right? Why, why did you choose choice (a)?

**P:** The concentration of reactants and products equal if  $\underline{K=1}$  that's what it reads, so when by definition <u>K is equal to 1</u>, when the <u>concentration of products and reactants is</u> <u>the same</u>, well, it's the same, yeah, it's the same, cuz it's products over reactants and so when you divide the top by the bottom, you get 1, so K equals to products over reactants

#### Student 2

*R*: *okay for #3, you choose (a). why did you choose that?* 

**P:** Okay, Umm, you know, I know, when I was thinking of equilibrium, <u>I was thinking of</u> equal, you know cuz K = 1.

**R**: Yeah so that's why you choose to go with (a)?

**P:** Yeah, it kinda makes sense

66% of students in the experimental group who answered item #5, held an algorithmic view, a common alternate conception, i.e., concentration of NO and NOCl at equilibrium must be equal because they existed in a 2 to 2 stoichiometry. Bilgin (2006) suggested students appeared to have memorized the taught rule and then tried to apply it without understanding the processes, fixating on the pervasive set of reasoning rule-rote recalling algorithm. In particular for items 5, the misconception was found to stem out based on consideration of co-efficients in a chemical reaction. The development of this misconceptions can be attributed to considerable emphasis placed on reaction stoichiometry in introductory topics Hackling and Garnett (1985) and Hameed et al (1994).

Representative transcribed student responses are shown below. The underlined words suggest the students were merely applying an algorithmic approach while solving the question.

In the first response shown below, while the student had the correct reasoning

(i.e., equilibrium will not shift towards either left or right, unless an external agent is

introduced) to eliminate choice c, the student incorrectly applied stoichiometric principles

in an algorithmic fashion to arrive at the final answer.

Student 1

**R**: Okay for #5, you choose (b) right, so what there a particular reason why decide to go with (b)?

*P*: *Cuz*, <u>NO and NOCl exists in a 2 to 2 stoichiometry, there will be equal amount of NO</u> <u>and NOCl</u>, stoichiometrically we say that for every amount of NO, we have at a same constant ratio the amount that's on the right which is NOCl

**R**: So why can't it be (c)?

**P**: (c) reads equilibrium shifts to the right, hence more NOCl will be present, well at equilibrium, and there is no shifting, because you are not adding or subtracting anything, which is why

The follow student responses illustrate the algorithmic approach taken to solve the

question. The underlined words illustrate the algorithmic approach.

Student 1

*R*: So what was your choice behind (b) for #5?

*P*: [laughs], I thought about it, <u>equal amounts</u>, I just assumed it means moles, cuz the <u>2 to</u> <u>2 stoichiometry</u>, and I just choose that, it kinda made sense to me.

Student 2

*R*: #5, you choose *B*,

*P*: Whenever I looked at the equation, they both 2 in front of them, <u>so it's a 2 to 2 or 1 to</u> 1, so will be equal amounts of them.

Two of 15 student held correct reasoning on why they choose choice d for item 5. Representative transcribed student responses is shown below. The underlined words illustrate students' thought process while solving the question. Both responses suggest that the students were able to demonstrate the dynamic aspect of chemical equilibrium (indicated by a bold arrow) in Figure 8. It is evident from the response shown below that, the student took a systematic approach while solving the item. The student took each item choice evaluated it before moving to a difference item choice.

*R*: And, okay, lets go to #5. What was your reasoning behind your answer choice for #5? *P*: Well, then based on that assumption, <u>you can't really determine</u>, <u>if Cl2 is the limiting</u> <u>reagent based on the information given</u>, Well even if they are in 2 to 2 ratio, you still can't, I mean like I said for (a) <u>you cannot really determine without initial concentration</u>, so you really cant say that, at equilibrium NO is going to decrease or get lost. See, if its at equilibrium, it is going to stay at equilibrium, there is <u>nothing here to influence</u> it to shift either way. So Le Chatelier's principle does not apply here, so that's why I choose (d) none of the above.

For item 6, 6 out of 15 students held an algorithmic view (procedure ontological category) and 5 out of 15 students held a formulaic view (procedure ontological category), i.e., attempting to fit a scientific concept in to an incorrect formula. The algorithmic or formulaic view held by students concur with the view reported by Bilgin (2006). Bilgin (2006) suggested students learn the taught rule by heart and they try to apply it without understanding, fixating on the pervasive set of reasoning rule-rote recalling algorithm.

Representative transcribed student responses are shown below. The underlined words suggest the students were merely applying an algorithmic or formulaic approach while solving the question.

In the following responses, the student held a formulaic view, i.e., incorporating the stoichiometry of reactants and products in to an equilibrium expression.

Formulaic view

Student 1

*R*: So, let's go with #6, you choose (a)

*P:* well, I couldn't remember, <u>if it was like the rates equal or if it was the concentration</u>. I thought of the <u>equilibrium expression</u>, <u>concentration of products over reactants</u>, so I know its concentration not rates

Student 2

R: So for #6, at equilibrium you choose B.

P: This is going to back to what I was saying for #3, where K =1, <u>because there is two</u> <u>moles of products and 3 moles of reactants, so K must be less than 1.</u> So I guess I got three wrong. I am thinking now, it must be none of the above for #3.

In the representative response below, the student demonstrates holding an

algorithmic view, i.e, applying the symbolic meaning of an equilibrium constant (K = 1)

to solve the item.

Algorithmic view

Student 1

*R*: What was your reasoning behind #6?

*P:* Ummm, I guess, I wasn't exactly sure about the question, if concentration of reactants and products are equal, then K's gotta be 1

For item 9, 93% of students in the control group held the common misconception, i.e., when a system at equilibrium is disturbed by a decrease in the volume of the system, rate of the forward reaction increases and rate of the reverse reaction decreases. The alternate conception is indicated by dotted arrow between the CBI (Reaction rate) and chemical equilibrium in Figure 8. Hackling and Garnett (1985) suggested this misconception was caused by students believing that reaction rates adjusted to facilitate the predictions made using LCP. Similar findings were reported by Cheung (2004). While the participants were teachers and the chemical system considered was different from the one considered in the current study, the findings concur with reasoning suggested by Hackling and Garnett (1985). More than 50% of teachers who participated incorrectly applied LCP to make predictions about the reaction rate when the volume of a system is decreased. Only 2 out of the 33 had valid scientific reasoning behind their answer choice.

The following representative interview responses reflect reasoning suggested by Hackling and Garnett (1985). The participants have made use of Le Chatelier's principle to make predictions about the reaction rate. While the students were able to understand the relationship between pressure and volume, the understanding was not extended to relate volume to molar concentration.

#### Student 1

#### P: Ummm, [long pause], well I had to think about this one

**R**: No problem, take your time

*P*: Well, you decrease volume, so you increase pressure, so it will move to right, so reaction cannot move to left, so, it's like, the<u>, the forward should increase and reverse should decrease</u>

*R:* You mean the rate?*P:* Yeah that's what I meantStudent 2

*R*: What was your reasoning behind #9? Initially, means right at the moment, when you make a change?

*P:* Let's see, {long pause], at that moment, yeah, when you constrain the volume, the forward reaction is going to go much faster, as it wants to re-establish equilibrium. Like I said if you decrease or constrain volume, its going to favor the side with least moles, so the forward reaction will increase and the reverse reaction will decrease.

Lastly, for items 11, 10 out of 15 students held a procedural view, i.e., incorrect application of Le Chatelier's principle while solving the item. Cheung (2009) emphasized that instruction does not focus on what happens to the system when it re-attains equilibrium. Rather the instruction focuses on direction of equilibrium shift. Providing students with a table that lists equilibrium shifts under different conditions, incorporates an algorithmic view in the minds of students.

Representative transcribed student responses are shown below. The underlined words suggest the students held a procedural view while solving the item. It is evident in all three responses, students applied Le Chatelier's principle to determine equilibriums shift, even though the question specifically request them to determine concentration of reactants and products when equilibrium re-establishes.

#### Student 1

*R:* #11, what was your reasoning?

**P:** Whenever volume is decreased, the reaction will go towards the side with least moles, so, <u>the left side has 3 moles</u>, and the right side has 2 moles, and so after equilibrium has re-established, <u>the left side which was NO and Cl2</u>, the concentrations would be less, and <u>NOCl would be greater</u>, cuz there only 2 moles of it.

## Student 2

*R*: Lets go to #11, what was your reasoning, as to why you decide to go with (f) for #11?

**P:** Okay, Ummm, [long pause], so, when you <u>decrease the volume</u>, I think it goes back the <u>products are favored</u>, so to re-establish equilibrium, it has to go in the reverse order, so it's going to use the <u>NO and Cl2</u>, so that's why they are less and the NOCl is greater.

**R**: Is there a principle did you use while answering the question?

**P:** Yeah I used the <u>Le Chatelier's principle</u> to determine the answer to this question

# Student 3

**R:** so what was your reason behind F for #11

P: Its kind of a process of elimination. But you know you could eliminate g and h.

**R**: You did decide to go with F.

P: I guess if you assume if it shifts to the right, less of the reactants and more of products.

## **Research Question 3: What evidence is observed to suggest changes in students' mental models on chemical equilibrium after they use the chemical equilibrium simulations?**

According to Chi (1994), conceptual change occurs when a concept is reassigned from one category to another. She asserts that all entities belong to one of the three ontological categories; a) entities, b) process and c) mental States. According to Chi's conceptual change model, a concept such as chemical equilibrium contains constraint based features like randomness, simultaneous, uniform activities. A constraint based interaction (CBI) provides no information about its time course, because it has no time course. The constraint based features might prevent students from deeply understanding the concept of chemical equilibrium. Concepts associated with chemical equilibrium such as rate of a reaction, molar concentration, equilibrium constant are also part of the CBI category. CBI and events are sub-categories of the event ontological category. Examples of events include; a reaction is dynamic or static, a reaction is happening in one direction, a reaction is happening in both direction. If a student add or delete concepts with in an event or CBI category, a basic conceptual change is achieved. If a student's thought process switches from an event sub tree to a CBI sub tree or switches from a matter to process category then a radical conceptual change is achieved.

For item 3, 14 of the 15 participants in the experimental group held a system view of chemical equilibrium post intervention. A higher percentage of students held a procedural view (information recall, algorithmic or formulaic view) of chemical equilibrium. Representative transcribed student responses is shown below. The underlined words suggest the students' mental model has changed for item post

intervention. Item 3 describes how the rate of a reaction occurs in a system at equilibrium. Hence, the concept of dynamic nature is important while understanding the concept of rate. Post intervention, not only did students had a stronger conceptual understanding of the rate concept, but also held a dynamic view. The change in ontological category from (procedural such as information recall) to CBI ontological category (Reaction rate) indicated by a blue arrow (Figure 9) running through the event ontological category (dynamic). Based on the Chi's (1994) ontological model, for item 3 a radical conceptual change has been achieved among students in the experimental group.

It is evident in the responses shown below, the students held a different model. In contrast during the pre-test, students held the belief that equilibrium refers to equal concentration, because K = 1 refers to a system attaining chemical equilibrium. This condition was described by Schafer (1984). The preconception of *equilibrium* stems from the idea used in everyday life, where equilibrium means equality of two sides, stability and static in nature (Schafer, 1984). While systems that reach chemical equilibrium may appear macroscopically stable and static, microscopically the system is dynamic not only because of molecular movement but also because the process of bond breakage and creation goes on. Equilibrium constant is defined as the ratio of concentration of products to reactants.

Student 1

**R**: Okay for #3, you may have changed your answer, that does not mean it's right or wrong? For # 3 you choose (a), on your post-test you decide to go with (c), why is that?

**P:** I kinda realize, after seeing the graph, <u>the reactants aren't going to be the same at</u> <u>equilibrium</u>, so K very might well equal 1, not because products, I mean concentration of products and reactants may not be the same, its just K expression is equal to 1, because its

**R**: So why do we say K equals 1. I mean, I really understood your logic, If in algebra we say, the ratio equals 1, what do we assume?

*P*: Well, if you assume, your ratio is 1, you have the same amount on one side and the same on the opposite side.

**R**: So if we say its constant as in (c), right, but we say equilibrium means K equals 1, what are we really refer to, these two cannot be equal, than how can K be equal to 1?

P: I would say the ratio of going from one end to the other is the same

*R*: so what is that ratio called?it's called by a different name.

P: May be rate?

Student 2

*R*: So there's shift on #3, you had (a) on the pre-test and on the post you have C, what was the reasoning behind your shift?

*P:* Well, again, the program clearly showed, like the pulley system, it showed, how if you add the weight, <u>the ratio is constant, it's a constant thing, whenever it reaches</u> <u>equilibrium</u>

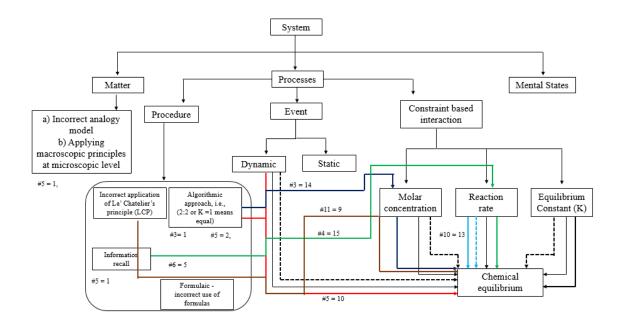


Figure 9: Coding taxonomy demonstrating mental model held by student's in the experimental group during the post-intervention phase.

For #4, none of the 15 participants in the experimental group held an algorithmic or formulaic or information recall (procedural ontological category) post intervention. Representative transcribed student responses is shown below. The underlined words suggest the students' mental model has changed for item post intervention. Item 4 describes how the rate of a reaction occurs in a system at equilibrium. Hence, the concept of dynamic nature is important while understanding the concept of rate. Post intervention, not only did students had a stronger conceptual understanding of the rate concept, but also held a dynamic view. The change in ontological category from (procedural such as information recall) to CBI ontological category (Reaction rate) indicated by a green arrow (Figure 9) running through the event ontological category (dynamic). Based on the Chi's (1994) ontological model, for item a radical conceptual change has been achieved.

#### Student 1

**R**: Okay for #4, you went with (b) on your pre-test and this time around you decide to go with (f), what was your reasoning?

P: Cuz, once its done

**R:** You mean it attained equilibrium

P: Yeah, that's what I mean

*P:* I mean, once its done, <u>its basically gonna be levelled out, that's what, I get it now,</u> <u>when it meant by constant over time,</u> that's why I decide to with (c), this time around.

*P*: *I* can also see, <u>the reaction continue to occur</u>, so (f) makes the most sense

R: Very good, good

#### Student 2

*R:* #4, you initially had g, this time you decide to with f, why is that?

**P:** Umm, I didn't really understand the concept of rate, I mean equilibrium rate at first, I kinda thought, <u>I actually mixed up concentration and rate. Now I understand now, at equilibrium, in order for it to be at equilibrium, the rates must be equal and then</u>

**R**: You also have chosen (C), does rates have to be constant or not necessarily?

P: I think it has to be both constant and equal

P: <u>I think the simulation made that concept much clearer</u>

#### Student 3

**R**: You also had change of answer for #4. Why did you change your previous answer choice on the pre-test?

**P:**[laughs], yeah, its kinda the same thing, like, the constant over time part, well I didn't really catch that the first time when I took the pre-test, but then when I did the program, it made me realize what the right answer was

*R*: Well now you know something about the rate and concentration at equilibrium *P*: [laughs], yeah

For #5, 10 of the 15 participants in the experimental group held a system view of chemical equilibrium post intervention. 40% of students in the experimental group held a procedural view (information recall, algorithmic or formulaic view) of chemical equilibrium. Representative transcribed student responses is shown below. The underlined words suggest the students' mental model has changed for item post intervention. In addition to stoichiometry and concentration, Item 5 describes how the rate of a reaction occurs in a system at equilibrium. Hence, the concept of dynamic nature is important while understanding the concept of rate. Post intervention, not only did students had a stronger conceptual understanding of the rate concept, but also held a dynamic view. The change in ontological category from (procedural such as information recall) to CBI ontological category (concentration, reaction rate and equilibrium constant) indicated by a red arrow (Figure 9) running through the event ontological category (dynamic). Based on the Chi's (1994) ontological model, for item a radical conceptual change has been achieved.

In the response below it is evident that the student not only was able to move away from an algorithmic perspective, but also held a dynamic view of the system

#### Student 1

**R**: Okay #5, you indicated a (b) on your pre-test, this time you decide to go with (d) why is that?

**P:** Again, because NO and NOCl exists in a 2 to 2 stoichiometry, <u>there won't be equal</u> <u>amounts of NO and NOCl</u>. I think the visual part of the thing, it was, it is, it really helped me to understand what the concentrations would be. Concentrations of NO, Cl2 and NOCl did not go to one thing, it were, it was, you know, <u>NO was its one thing</u>, <u>Cl2 was its</u> <u>one thing</u> *R*: Okay, will it ever be the same? Under any circumstances would it ever be the same? Can we say that? If it's not equal, what makes it that way?

*P:* Because <u>equilibrium is dynamic</u>, <u>when you change one thing, in this case if you</u> change NO, you change two others, so I think that's probably why

In the response below it is evident, the student has moved away from the

algorithmic approach to a system view of chemical equilibrium.

Student 2

R: Okay for #5, you had (c) for your pre-test, and you decide to go with (d) for the post-test. What was the reason behind that?

P: Well the first time around, I didn't even pay attention to C, I only read the equilibrium shift to right. Well from the graphs I can tell NO and NOCl were not equal, so that's why I eliminated B, A its obvious, as the simulation showed Cl2 was left in the container.

P: Well I also that you underlying words was helpful. It just made me think a little better.

For item 10, 13 out of 15 students in the experimental group held correct conception about rate of a reaction when a system at equilibrium is disturbed by a decrease in the volume of the system. Before the intervention, a higher percentage of students held the misconception, rate of the forward reaction increases and rate of the reverse reaction decreases. Hackling and Garnett (1985) suggested a possible reason behind this misconception. The misconception was caused by students believing that reaction rates adjusted to facilitate the predictions made using LCP. The alternate conception is indicated by dotted light blue between the CBI (Reaction rate) and chemical equilibrium in Figure 9. The correct conception post intervention is indicated by the solid light blue arrow between the CBI (Reaction rate) and chemical equilibrium in Figure 9. Because students only added a new concept and deleted an existing concept with in ontological tree, the resulting conceptual change is a basic conceptual change. Representative transcribed student responses is shown below. The underlined words suggest the students' mental model has changed for item post intervention.

In both responses shown below it is evident, the students have moved away from the reasoning suggested by Hackling and Garnett (1985). The underlined words suggest that the students hold a system's view, i.e., if you decrease volume of the system, concentration of all species would go up because molar concentration is the ratio of moles of solute over total volume of the system.

## Student 1

**R**: For #10, you indicated (c) as your choice, this time you decide to go with (f), what was your reasoning behind the change?

**P:** Okay when new equilibrium is re-established after decreasing the volume, which means you increase the pressure, <u>rates of forward and reverse reaction will be greater</u> <u>than before</u>, so,

**R**: Why do you think its greater?

*P*: Rate = k\*times.

P: I don't think that's right,

R: No go ahead and complete it, this is one way of writing it

**R**: So how did we define rate earlier in our interview?

**P:** We said concentration over time

**R**: Why do you think rate is greater, what made rate greater?

*P: more stress on reactants and products, to compensate, subsequent increase in NOCl, there is also going on in the reverse direction,* 

**R:** So what is increased in the ratio?

P: <u>The concentration of the products and the reactants</u>?

#### Student 2

# *R*: Okay for #10 you had (C) and for your post-test you have (f), why is that? *P*: <u>Whenever the volume is decreased, it's gonna be higher concentration, so, both the</u> rates are going to increase, in order for equilibrium to form again.

Lastly, for item 11, 9 out of 15 students did not hold a procedural view, i.e., incorrect application of Le Chatelier's principle while solving the item. The primary reason behind this alternate conception was described by Cheung (2009). Cheung (2009) emphasized that instruction does not focus on what happens to the system when it reattains equilibrium. Rather the instruction focuses on direction of equilibrium shift. Providing students with a table that lists equilibrium shifts under different conditions, incorporates an algorithmic view in the minds of students. Representative transcribed student responses is shown below. The underlined words suggest the students how students have moved away from a procedural view to a system view by including the effect of volume towards an increase in molar concentration of all species contained in the system. The shift from a procedural to a CBI category is indicated by a brown solid arrow shown in Figure 9. The arrow runs through both the dynamic event category and the molar concentration (CBI) category.

The question towards which participants showed least improvement has been item #6. Similar results were seen during the pilot study. The researcher was able to identify three potential reasons from participant responses during the pre and post-qualitative interview responses. The first being a) student responses showed ambiguity over the understanding of an equilibrium constant. Students who choose insufficient information has the option held this view. Following transcribed student response demonstrates a

participant's view towards choosing insufficient information

*R*: So, its very interesting, on #6, you decide to go with a, and then but this time you decide to go with none of the above

**P:** I thought of the lab we just did, I remember like finding the equilibrium constant, and then I realized, each reaction has its own K, its not necessarily equal to K, so any of these can be right.

**R**: The reason I picked 6 is, because for 3 you choose C, now if you had chosen a for 6, wouldn't that be contradicting? Cuz constant does not mean equal to one.

**P:** I thought about d, its rate of the reaction, I wasn't sure if it was rate of formation, I thought K had its own specific value.

*R*: Well you have a good point, cuz students are not really told, what K = 1 really implies

b) the second being, the fact, participants who answered item #3 and #4 correctly on the post-test, still held the view, K=1 implies concentration of reactants and products are equal. This is in direct contradiction to an answer choice for #3, concentration of reactants and products remain constant and answer choice for #4, rates of the forward and reverse reactions are equal at equilibrium. Following transcribed student responses demonstrates a participant's view towards choosing the choice, K=1 because concentration of reactants and products are equal

Student 1

**R:** So, let's go with #6, you choose (a)

**P:** well, I couldn't remember, if it was like the rates equal or if it was the concentration. I thought of the equilibrium expression, concentration of products over reactants, so I know its concentration not rates

**R:** What was your reasoning behind #6?

**P:** Ummm, I guess, I wasn't exactly sure about the question, if concentration of reactants and products are equal, then K's gotta be 1

## Student 2

**R:** What was your reasoning behind #6?

**P:** Ummm, I guess, I wasn't exactly sure about the question, if concentration of reactants and products are equal, then K's gotta be 1

c) third being, students lacked a conceptual understanding about the meaning of K. As discussed above, it is quite interesting that students were able to secure correct response and corresponding correct reasoning for item #3 and #4, they were not able to extend the knowledge to item #6. Partly the issue is due to overemphasis of mathematical calculations involving equilibrium constant (K) during instruction.

# **Research Question 4: What are students' conceptions of chemical equilibrium after interacting with the simulations?**

Following graphical representation Figure 10 compares the percentage of misconceptions held by participants in both groups during the pre-phase and what percentage of those misconceptions have been corrected during the post-phase.

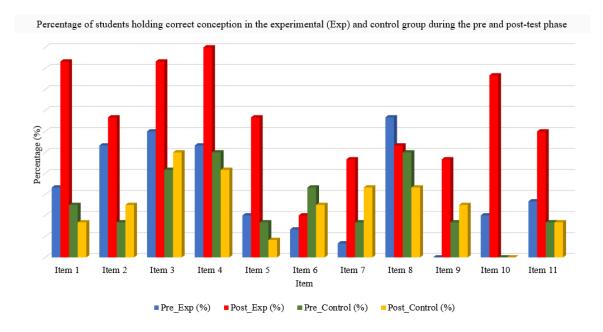


Figure 10: Graphical representation of the percentage of correct conception held by participants in the control and experimental groups during the pre and post phase

Results of the study provided positive outcomes and justified the purpose of the study in the first place. The following items recorded the higher percentage (shown in parenthesis as pre %, post %) of correct response from students in the experimental group. Item 1 (33%, 93%), Item 3 (60%, 93%), Item 4 (53%, 100%), Item 5 (20%, 67%), Item 7 (7%, 47%), Item 10 (20%, 87%), Item 11 (27%, 60%). Participants registered marginal gains with items 6, 8 and 9. Visualization through simulation provides a

promising approach to the widespread problem of misconceptions and the need for challenging instruction to be specific and definitive for each particular misconception. That is, those students who received the experimental intervention had exceptionally higher conceptual understanding of chemical equilibrium concepts.

## **Connections to the Multimedia Framework**

The Schnotz integrated framework was chosen as the multimedia framework for the current study. The cognitive architecture of the model consists of working memory, sensory registers and long term memory In addition the model's architecture consists of a cognitive level and a perceptual level. A major difference between the model presented under the cognitive theory of multimedia learning and the current model is the former model assumes independent construction of a verbal mental model and pictorial model which then later have to be integrated. The current model proposes that only one mental model is constructed that integrates information from different sources right from the start. Most, if not all students, found the visual image more helpful over the audio component. They constructed a single mental model based on the pictorial information alone. It was very much evident from response, especially among participants who failed to choose a correct answer choice for #1, #2 and #3. In addition to the visual component, the audio component reinforced the concept.

Participants attributed the visual component was predominantly helpful towards developing conceptual understanding over the audio component. While all participants

found the audio helpful as it assisted them with their conceptual understanding, they admitted it was the visual aspect of the graphs that immediately grabbed their attention.

## **Implications and Ideas for Future Research**

Results of the study provided positive outcomes and justified the purpose of the study to explore the effectiveness of a simulation to support students' conceptual understanding of chemical equilibrium. Statistical significance from the independent samples t-test suggests that the intervention has played a key role in students' conceptual understanding of chemical equilibrium concepts presented in the study. A reliability of alpha = 0.71 for the quantitative CEMT instrument supports the reliability of the instrument used. This instrument was constructed in order to assess change in participants' conceptual understanding of chemical equilibrium. The two-tier instruments (Ozmen, 2008 & Treagust, 2015) described in Chapter 2 focused on a wide variety of chemical reactions. Whereas, the instrument developed for the current study maintained a narrow focus to address chemical equilibrium as it was presented in the simulations. Prior instruments developed by Hackling and Garnett consisted of true or false items, hence the current instrument offered more detail to identify students' misconceptions of chemical equilibrium concepts. The instrument could be used by science education or chemical education researchers exploring the domain of chemical equilibrium misconceptions. The simulations developed and used in the research study will not be available to members of the research and public domain as corrections suggested by students in the experimental group had to be made.

205

The study also did not focus on other areas of chemical equilibrium misconceptions such as effect of temperature, catalyst or addition of inert gas. While simulations were created to address these misconceptions, due to time constraints they were left out from the study. The simulations were designed to explore these ideas, but again due to time constraints, they were not pursed. Research studies have explored student misconceptions in areas of chemistry such as gas laws, stoichiometry and chemical kinetics. One of the primary reasons behind students' lack of conceptual understanding towards chemistry concepts in general is, that they learn concepts in a segregated manner. In other words, students learn concepts such as stoichiometry, gas laws during the first semester and learn advanced concepts such as chemical kinetics, thermodynamics and equilibrium in the second semester.

Segregation of instruction leads to a compartmental view of chemistry concepts among students. It was very much evident from participant responses in current research study that participants fragmented understanding of the concepts of rate (Kinetics); moles (stoichiometry); and the relationship between moles, volume and concentration (gas laws and stoichiometry). The study provided a snapshot into the effect of visualization tool such as simulation towards student's conceptual understanding of chemical equilibrium concepts. Future studies are needed to explore how simulations similar to the set used in the current study can be used to support student learning of gas laws, stoichiometry, and kinetics before presenting simulations related to chemical equilibrium. Such studies might uncover conceptual difficulties students experience in learning these concepts, and how a series of simulation modules could be used to deepen students' understanding of the foundational concepts and of chemical equilibrium.

206

Appendices

## APPENDIX A

# CHEMICAL EQUILIBRIUM MISCONCEPTIONS TEST (CEMT)

## **CEMT Instrument**

Name \_\_\_\_\_

**Questions 1-11** are based on the following reaction.

 $2NO(g) + Cl_2(g) \implies 2NOCl(g) + heat$ 

- 1. As the reaction approaches equilibrium,
- a) The rate of forward and reverse reactions increase at the same rate
- b) The rate of forward reaction increases as the reaction gets going
- c) The rate of the forward reaction decreases as the reaction gets going
- d) Reverse reaction rate is same as the forward rate as the reaction gets going
- e) The rate of forward and reverse reactions decrease at the same rate as the reaction gets going
- f) None of the above
- 2. As the reaction approaches equilibrium,
- a) Concentration of reactants and products is equal because K=1
- b) Concentration of reactants is 3 times more than concentration of products
- c) Concentration of reactants is 3 times less than concentration of products
- d) Concentration of reactants and products is constant because K<1
- e) None of the above

#### 3. At equilibrium,

- a) Concentration of reactants and products is equal because K=1
- b) Concentration of products is greater because K>1
- c) Concentration of reactants and products is constant over time
- d) None of the above
- 4. At equilibrium,
- a) Forward and reverse reaction continue to occur
- b) Forward and reverse rates are equal
- c) Forward and reverse reaction rates are constant over time
- d) Reverse rate is greater than forward rate, because reactants are lost and products are formed
- e) a & d
- f) a b & c
- g) a & c

- 5. <u>At equilibrium</u>,
- a) Because Cl<sub>2</sub> is limiting reagent, there will no Cl<sub>2</sub> left
- b) Because NO and NOCl exist in 2:2 stoichiometry, there will be equal amounts of NO and NOCl<sub>2</sub>
- c) Equilibrium shifts toward right, hence more NOCl will be present
- d) None of the above
- 6. At equilibrium,
- a) Equilibrium constant K = 1 because concentration of products and reactants are equal
- b) Equilibrium constant K < 1 because the total moles of products is less than total moles of reactants
- c) Equilibrium constant K>1 because reactants are consumed and more products are formed
- d) Equilibrium constant K =1 because rate of product and reactants formation is equal and constant over time
- e) None of the above
- 7. At equilibrium concentration of [NO] is <u>instantaneously</u> increased at constant volume,
  - a) Rate of reverse reaction will decrease because equilibrium shift towards right
  - b) Rate of forward reaction will increase,
  - c) Rate of reverse reaction will increase because more NOCl is formed
  - d) Rate of forward reaction will not change, because volume is constant
  - e) a & b
  - f) c & d
- 8. After addition of [NO], when new equilibrium is re-established,
  - a) The equilibrium constant K will be the same
  - b) The equilibrium constant K will be greater because [NOCl] is increased
  - c) The equilibrium constant K will be less because NO and  $Cl_2$  are lost
  - d) Insufficient information provided
  - e) None of the above

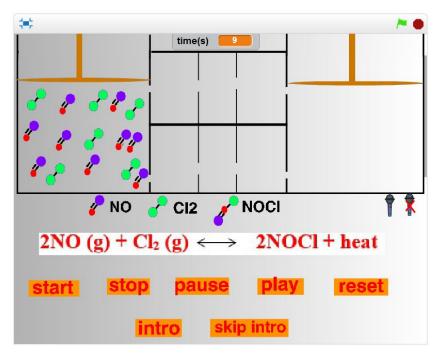
- 9. Equilibrium is disturbed by decreasing the volume at constant temperature, <u>initially</u>
  - a) Rate of forward reaction increases
  - b) Rate of reverse reaction decreases
  - c) a & b
  - d) Rate of reverse reaction increase
  - e) Forward reaction rate will be greater than reverse reaction rate
  - f) a & d
- 10. Equilibrium is disturbed by decreasing the volume at constant temperature, when <u>new equilibrium is re-established</u>
  - a) Rate of forward reaction increases
  - b) Rate of reverse reaction decreases
  - c) a & b
  - d) Rates of forward and reverse reaction will be equal
  - e) Rates of forward and reverse reaction will be greater than the initial equilibrium
  - f) d & e
- 11. Equilibrium is disturbed by decreasing the volume at constant temperature, when <u>new equilibrium is re-established</u>
  - a) Concentration of NO will be less in the new equilibrium compared to first equilibrium
  - b) Concentration of NO will be greater in the new equilibrium compared to first equilibrium
  - c) Concentration of Cl<sub>2</sub> will be greater in the new equilibrium compared to first equilibrium
  - d) Concentration of Cl<sub>2</sub> will be less in the new equilibrium compared to first equilibrium
  - e) Concentration of NOCl will be greater in the new equilibrium compared to first equilibrium
  - f) a, d & e
  - g) b, c & e
  - h) b, d & e

## **APPENDIX B**

# CHEMICAL EQUILIBRIUM SIMULATIONS

Simulation 2: The concept of chemical equilibrium – Microscopic view





At equilibrium

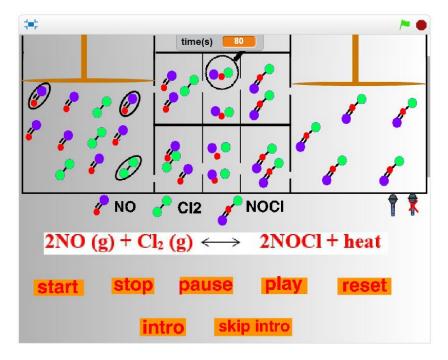
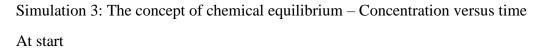
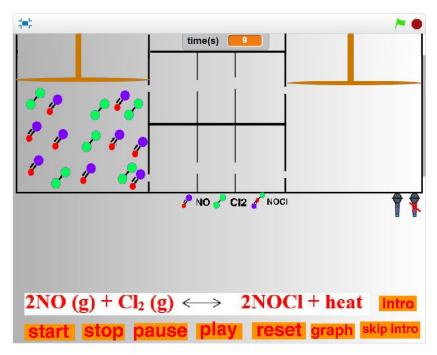


Figure 11: Simulation of a system attaining chemical equilibrium





At equilibrium

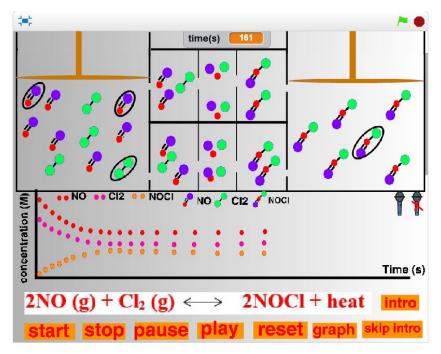
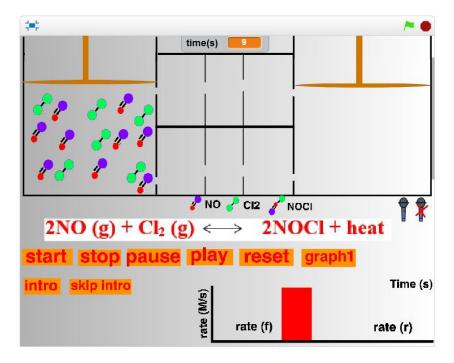


Figure 12: Simulation of a system attaining chemical equilibrium featuring concentration versus time graph

Simulation 4: The concept of chemical equilibrium – Rate of a reaction At start



At equilibrium

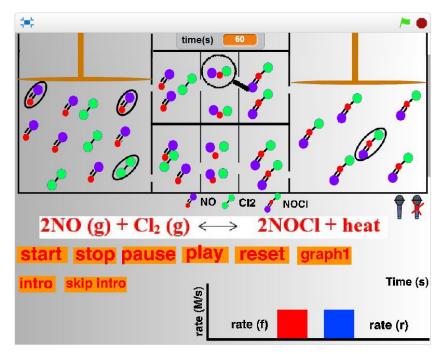
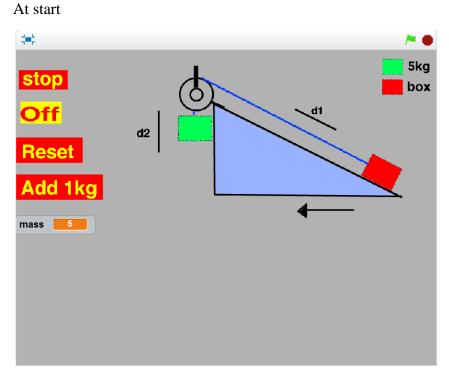


Figure 13: Simulation of a system attaining chemical equilibrium rate of a reaction in graphical form



Simulation 5: Pulley experiment – Analogy model

In the end

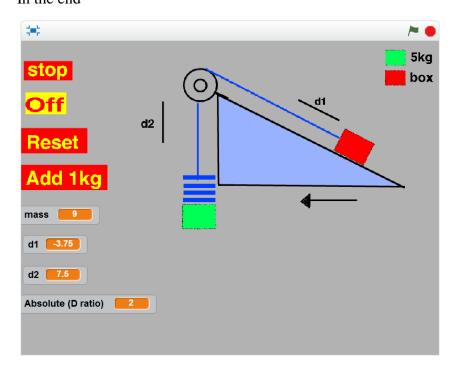
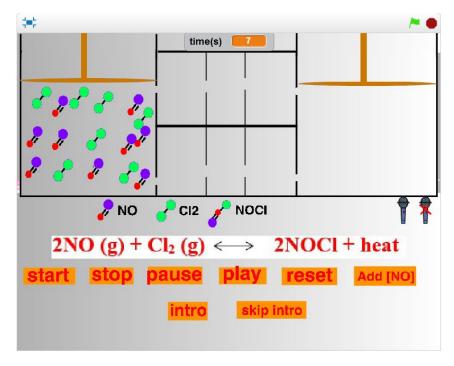


Figure 14: Pulley experiment

Simulation 6: Changing equilibrium conditions – Effect of concentration change At start



After addition of NO and equilibrium reestablishes

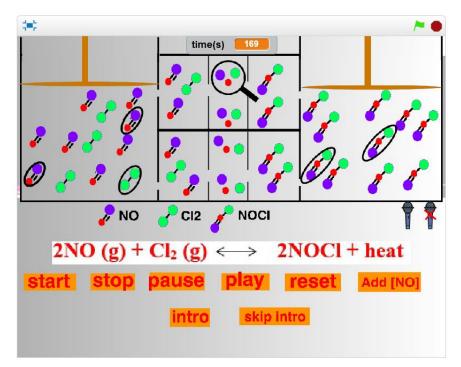
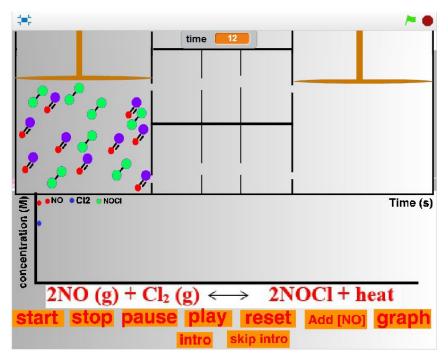


Figure 15: Changing equilibrium conditions by addition of NO

Simulation 7: Changing equilibrium conditions – Effect of concentration change (graphical)

At start



After addition of NO and equilibrium re-establishes

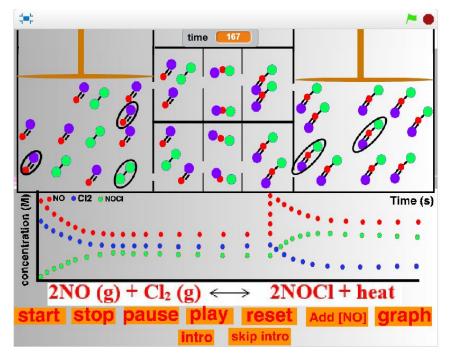
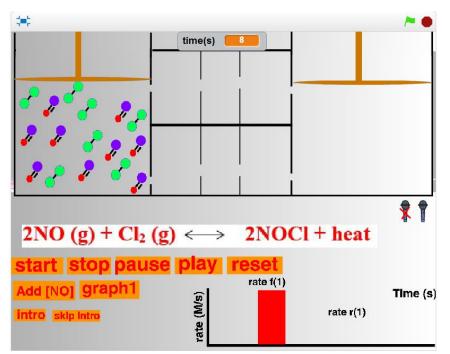


Figure 16: Changing equilibrium condition by addition of NO, graphical representation of concentration change as a function of time

Simulation 8: Changing equilibrium conditions – Effect of concentration change (graphical)

At start



After addition of NO and equilibrium reestablishes

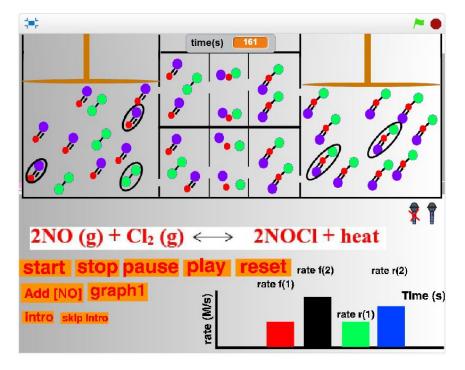
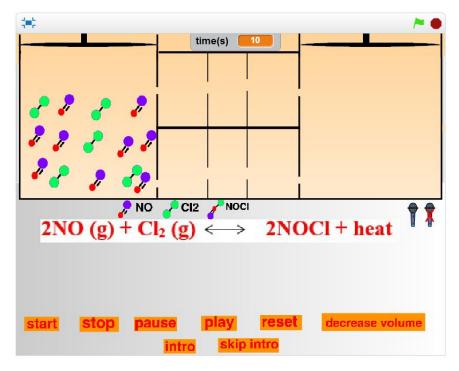


Figure 17: Changing equilibrium condition by addition of NO, graphical representation of rate of the forward and reverse reaction

Simulation 9: Changing equilibrium conditions – Effect of volume change At start



After volume is adjusted and equilibrium reestablishes

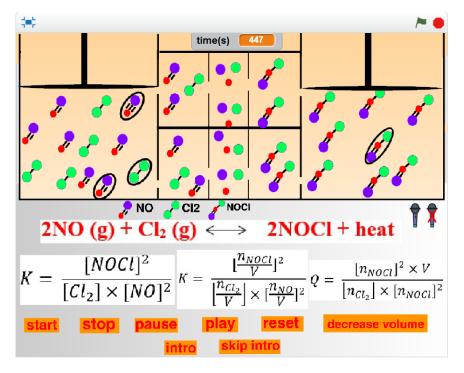
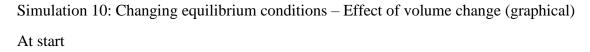
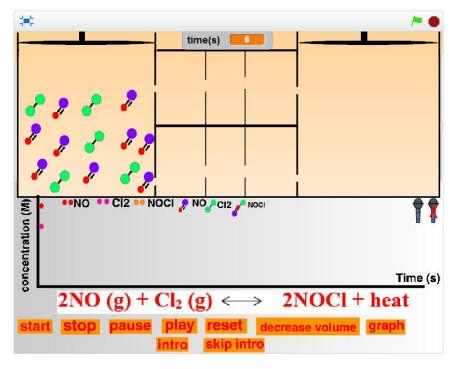


Figure 18: Changing equilibrium conditions by decreasing volume of the system





After volume is adjusted and equilibrium reestablishes

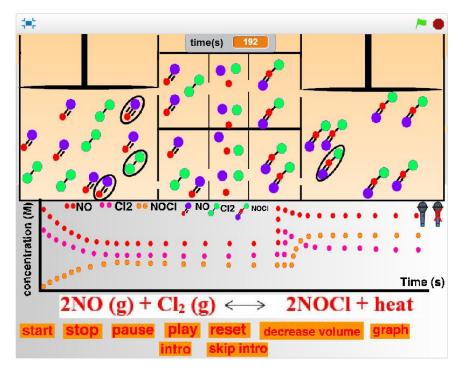
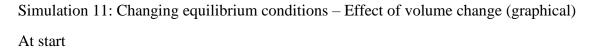
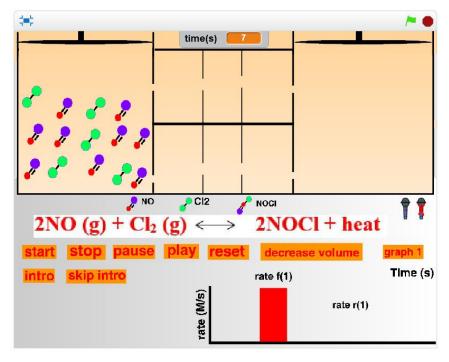


Figure 19: Changing equilibrium condition by decreasing volume, graphical representation of concentration change as a function of time





After volume is adjusted and equilibrium reestablishes

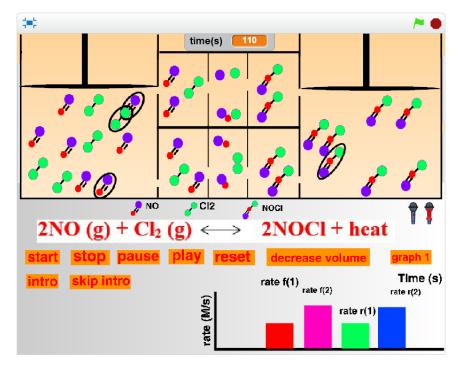


Figure 20: Changing equilibrium condition by volume change, graphical representation of rate of the forward and reverse reaction

## **APPENDIX C**

# QUALITATIVE DATA CODING

# Dissertation Study Experimental group\_PRE-TEST

Larger theme – Conceptual Understanding

\*Participants who answered none of the above or insufficient information provided are not included for analysis in the table, as they do not constitute a theme. In some cases none of the above or insufficient information is the correct answer\*

	Theme1 – Approaching Equilibrium				
	<b>Question 1:</b> As the reaction approaches equilibrium, in terms of rate? (N=15)				
N	Sub Themes	Concepts (vocabulary)	Student quotes		
	Theme 1(a)				
1	Rate of forward and reverse rates increase at the same rate				
	Theme 1(b)				
3	Rate of forward and reverse rate decreases at the same rate		E5: "Ummm, so, my thought process was that, I am thinking they had to have, not necessarily the same rate on both sides, but the rate changing at the same right?"		
	Theme 1(c)				
5	The rate of the forward reaction decreases	Rate, equal, decreases, less reactants, more products	E4: "as the reaction starts, its going to produce more and more products, but as it gets closer and closer to equilibrium, its going to produce less and less products"		
	Theme 1 (d)				

4	Reverse and forward rates are equal Theme 1 (e)		E3: "Ummm, what equilibrium, the forward reaction would go up and reverse reaction would go down, that what equilibrium is, if rate goes up, at least one of em has to go down"
2	Rate of forward reaction increases		E8: "because it
	Overtisen 2: As the most interpretent of the second interpretent of the sec		says it increases and I also saw release of heat, and whenever I put heat in to it, a reaction that's slower and the heat speeds it up"
N	<b>Question 2:</b> As the reaction approaches equilibr		
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 2(a)		
1			
	Concentration of reactants is 3 times less than concentration of products		
3			E3: "Most of these have like different ratio. It's like K is less than 1, it wants to be equal, so that's why I decide to go with (a)"
	concentration of productsTheme 2(b)Concentration of reactants and products is		have like different ratio. It's like K is less than 1, it wants to be equal, so that's why I decide

	moles of reactants, so, that's why"

	Theme 2 – Characterist	ics of Equilibrium	
	<b>Question 3:</b> At equilibrium, in terms of concen		
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 3(a)		
4	Concentration of reactants and products is equal because equilibrium constant K=1	Arithmetic, ratio, equilibrium means equal,	E1: "The concentration of reactants and products equal if K=1 that's what it reads, so when by definition K is equal to 1, when the concentration of products and reactants is the same" E14: "I have kind of remembered that K =1 is the goal to reach for equilibrium, it's like perfect equilibrium I think" E13: "I know, when I was thinking of equilibrium, I was thinking of equal, you know cuz K = 1"
	Theme 3(b)		

9	concentrations don't change over time		E2: "Ummm, equilibrium just means that, both forward and reverse reactions are happening at the same rate. So, the concentrations don't change otherwise"
	Theme 3(c)		
1	Concentration of reactants and products is greater, because K>1	Confused, unsure,	<b>E9:</b> "I didn't know anything about K for this reaction and I was honestly confused about that, so I started thinking, what if K is small or big, and I know when K is big, you are favoring the products"
	Question 4: At equilibrium, in terms of rate? (1	N=15)	
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 4(a)		
1	Forward and reverse reaction continue to occur		
	Theme 4(b)		
3	Forward and reverse rates are equal		E3: "I kinda wanted to choose (b), but I didn't see a choice with b & c, so I decide to go with just b"
	Theme 4(c)		
8	Forward and reverse reaction continue to		
	occur, rates are equal and constant over time		
	Theme 4(d)		
1	Forward and reverse rates equal and continue to occur		

Question 5: At equilibrium, in terms of stoichiometry? (N=15)       Student quotes         N       Sub Themes       Concepts (vocabulary)       Student quotes         6       Equal amount of NO and NOC1       Arithmetic, equal, stoichiometry       E1: "Cuz, NO and NOC1 exists in a 2 to 2 stoichiometry, there will be equal amount of NO and NOC1"         8       E4: "but yeah ,looking at the reaction, the stoichiometry is 2:2, you should say that under certain conditions, it makes sense"         8       E15: "Whenever I looked at the equation, they both 2 in front of them, so it's a 2 to 2 or 1 to 1, so will be equal amounts of them"	2	Forward and reverse reaction continue to occur and constant over time	Prior knowledge	E14: "So for (a) forward and reverse reactions continue to occur, I know at equilibrium, its going back and forth, For C, I saw constant in the questions, and I was thinking constant over time, that's why I choose C"
N       Sub Themes       Concepts (vocabulary)       Student quotes         6       Equal amount of NO and NOC1       Arithmetic, equal, stoichiometry       E1: "Cuz, NO and NOCI exists in a 2 to 2 stoichiometry, there will be equal amount of NO and NOCI"         6       Equal amount of NO and NOC1       Arithmetic, equal, stoichiometry       E1: "Cuz, NO and NOCI exists in a 2 to 2 stoichiometry, there will be equal amount of NO and NOCI"         6       E4: "but yeah, looking at the reaction, the stoichiometry is 2:2, you should say that under certain conditions, it makes sense"       E15: "Whenever I looked at the equation, they both 2 in front of them, so it's a 2 to 2 or 1 to 1, so will be		Question 5: At equilibrium, in terms of stoichi	ometry? (N=15)	
6       Equal amount of NO and NOCI       Arithmetic, equal, stoichiometry       E1: "Cuz, NO and NOCI exists in a 2 to 2 stoichiometry, there will be equal amount of NO and NOCI"         E4: "but yeah ,looking at the reaction, the stoichiometry is 2:2, you should say that under certain conditions, it makes sense"       E15: "Whenever I looked at the equation, they both 2 in front of them, so it's a 2 to 2 or 1 to 1, so will be equal amounts of	N	Sub Themes	Concepts	Student quotes
stoichiometryNOCl exists in a 2 to 2 stoichiometry, there will be equal amount of NO and NOCI"E4: "but yeah ,looking at the reaction, the stoichiometry is 2:2, you should say that under certain conditions, it makes sense"E15: "Whenever I looked at the equation, they both 2 in front of them, so it's a 2 to 2 or 1 to 1, so will be equal amounts of				
Theme 5(b)	6		-	<ul> <li>NOCl exists in a 2 to 2 stoichiometry, there will be equal amount of NO and NOCl"</li> <li>E4: "but yeah ,looking at the reaction, the stoichiometry is 2:2, you should say that under certain conditions, it makes sense"</li> <li>E15: "Whenever I looked at the equation, they both 2 in front of them, so it's a 2 to 2 or 1 to 1, so will be equal amounts of</li> </ul>

3	Equilibrium shifts toward right, hence more NOCl will be present	Analogy, additional components, arithmetic,	<ul> <li>E3: "I was think if you had 2 NO, I mean if you got 3 on the left side and 2 on the right side + heat, you kinda got this big slope, it just wants to bounce it out, its basically spilling all on the right side"</li> <li>E14: "I think it's the amount of products and reactants and it would shift to the side with the smallest number of stuff"</li> </ul>

	Theme 3 – Equilibrium Constant		
	Question 6: At equilibrium, what is true abo	ut equilibrium cons	tant?(N=15)
Ν	Sub Themes	Concepts	Student quotes
		(vocabulary)	
	Theme 6(a)		
5	Equilibrium constant (K) is less than 1		E15: "because there is two moles of products and 3 moles of reactants, so K must be less than 1"
	Theme 6(b)		
2	Equilibrium constant (K) is greater than 1		
	Theme 6(c)		

4	Equilibrium constant (K) is equal to 1, concentration of reactants and products are		<b>E12:</b> "if it was like the rates equal or
	equal		if it was the
			concentration. I
			thought of the equilibrium
			expression,
			concentration of products over
			reactants, so I
			know its
			concentration not rates"
			E11: "I wasn't
			exactly sure about the question, if
			concentration of
			reactants and products are equal,
			then K's gotta be
			1"
	Theme 6(d)		
2	Equilibrium constant $K = 1$ , because forward and reverse rates are equal		
	<b>Question 8:</b> After addition of [NO], when new	v equilibrium is re-es	tablished? (N=15)
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 8(a)		
5	Equilibrium constant greater than 1	Arithmetic, ratio, more versus less,	<b>E3:</b> "I was still thinking of the 1 to
		co-efficients,	1 ratio, since we
		prior knowledge	are adding more, it
			can now become a 2 to 2 or even a 3
			to 3 ratio? It's still
			the same, its just a lot greater than
			before"
			<b>E14:</b> "I was
			thinking, trying to
			remember prior
			knowledge, about

		<ul> <li>what we learned in class, we learned a few tricks, like, more products added, the K go this way, whatever and took a guess, if you add more reactants, it shifts to the products"</li> <li>E4: "the concentration of NOCI is going to be greater in the newer equilibrium, so your concentration of the products will be higher, and reactants will be lower, so that would create a bigger constant K"</li> </ul>
	Theme 8(b)	
10	Equilibrium constant is the same	<b>E9:</b> "I mean the initial concentration does not affect K, so that's why I picked that one"

	Theme 4 – Changing equilibrium conditions		
	<b>Question 7:</b> At equilibrium concentration of [NO		
	volume (N=15)	I	I
Ν	Sub Themes	Concepts	Student quotes
		(vocabulary)	
	Theme 7(a)		
1	Rate of forward reaction will instantaneously		
	increase		
	Theme 7(b)		
	Rate of reverse reaction will gradually increase		
	Theme 7(c)		
13	Rate of reverse reaction will decrease and		E2: "NO is on the left side of the
	forward rate will instantaneously increase		
			equation, when you disturb the
			equilibrium, it will try to go back to
			equilibrium, it tries
			to reach that ratio
			again, since it now
			has a greater
			amount on the left
			side, will try to
			convert that to
			substance on the
			right side, because
			of that (a) rate of
			the reverse reaction
			will decrease,
			because equilibrium
			shifts to right. and
			(b) makes sense has
			forward reaction
			rate will be
			increase"
			E5: "my thought
			was, rate of the
			reverse reaction
			will increase,
			because we add
			more NO, you will
			go this way, so that
			was the reason"
	Theme 7(d)		

1	Rate of reverse reaction will increase, because more NOCl is formed		E3: "If you put NO, it should shift towards right, kinda sounds like (a), the only thing I probably should have thought about is, what it meant by rate of reverse reaction going up"
	Question 9: Equilibrium is disturbed by decreas	sing the volume at co	onstant temperature,
N	initially? (N=15) Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 9(a)		
7	Rates of forward reaction increase, reverse reaction decrease		<ul> <li>E7: "Like I said if you decrease or constrain volume, its going to favor the side with least moles, so the forward reaction will increase and the reverse reaction will decrease"</li> <li>Well, you decrease volume, so you increase pressure, so it will move to right, so reaction cannot move to left, so, it's like, the, the forward should increase and reverse should decrease</li> </ul>
	Theme 9(b)		
3	Rate of forward reaction increase		
	Theme 9(c)		
1	Rate of reverse reaction decrease		
	Theme 9(d)		
2	Forward reaction rate will be greater than reverse reaction rate		
	Theme 9(e)		

2	Rate of forward reaction increases, reverse rate		
2	decreases and forward rate greater than reverse		
	_		
	rate	ing the velume of ee	actant tampanatura
	<b>Question 10:</b> Equilibrium is disturbed by decreasing the volume at constant temperature, when new equilibrium is re-established (rate) $(N=15)$		
NT			
Ν	Sub Themes	Concepts	Student quotes
		(vocabulary)	
2	Theme 10(a)		
2	Rate of forward reaction increase and		
	Rate of reverse reaction decreases		
-	Theme 10(b)		
3	Rate of forward and reverse reaction are equal		
	and greater than the first equilibrium		
	Theme 10(d)		
1	Rate of forward and reverse reaction will be		
	greater in the newer equilibrium		
	Theme 10(e)		
8	Rate of reverse reaction increases		
	Theme 10 (f)		
1	Rate of Forward and Reverse reactions are		<b>E9:</b> "I think it
	equal		should be F, cuz if
			the volume is
			decreased, there is
			going to be more
			particle movement,
			so the rate of the
			reaction will be
			faster. But then it
			will also be equal.
			There is increased
			pressure"
	Question 11: Equilibrium is disturbed by decreasing the volume at constant temperature,		
	when new equilibrium is re-established (concentration) (N=15)		
Ν	Sub Themes	Concepts	Student quotes
		(vocabulary)	
	Theme 11(a)		

10	Concentration of NO and Cl2 will be less and NOCl will be greater in the newer equilibrium	Le Chatelier's principle, algorithmic, guess work, process of elimination	<ul> <li>E1: "So you go to the side with the least amount of stress, so we go to right, going to (d), we have the concentration of Cl2 will be less than first, and the concentration of NOCl would have to increase as in (e)"</li> <li>E13: "Umm, there's less concentration of some of these, so I choose b &amp; d which is less and then I am not sure with e, I guess it's gotta be greater"</li> </ul>
-	Theme 11(b)		
4	Concentration of NO, Cl2 and NOCl will be greater in the newer equilibrium		E2: "Ummm, the concentrations of the substances in the solution are greater, concentration is the measure of the amount of the substance over volume, if volume is lower then concentration must be higher"
1	Theme 11(c) Concentration of NO, NOCl will be greater and		
1	Cl2 will be less in the newer equilibrium		

### **Dissertation Study Experimental group\_POST-TEST**

Larger theme – Conceptual Understanding

\*Participants who answered none of the above or insufficient information provided are not included for analysis in the table, as they do not constitute a theme. In some cases none of the above or insufficient information is the correct answer\*

	Theme1 – Approaching Equilibrium		
	<b>Question 1:</b> As the reaction approaches equi		rate? (N=15)
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 1 (a)		
14	The rate of the forward reaction decreases		E13: "Well, cuz, on the program it showed, the rate of the forward reaction decreases as it gets going"
			<b>E11:</b> "Ummm, I guess, I saw on the simulation, its kind of obvious, the rate of the forward reaction decreased as the reaction starts happening"
	Theme 1 (b)		
1	Reverse and forward rates are equal		E12: "I remembered my professor saying, at equilibrium the reaction rates are equal"
	<b>Question 2:</b> As the reaction approaches equi (N=15)	ibrium, in terms of c	
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 2(a)		
1	Concentration of reactants and products is equal, K=1		
	Theme 2(b)		

3	Concentration of reactants is 3 times more than concentration of products	E5: "I thought about it, but it looks right"
	Them 2(c)	
1	Concentration of reactants and products is constant, because K < 1	E4: "So, when I thought of the question, I immediately thought of the visual, it was not constant and when it got to equilibrium, it remained constant, like the entire time, so I automatically thought of that when I answered the question"

		ristics of Equilibriun	1	
	Question 3: At equilibrium, in terms of concentration? (N=15)			
N	Sub Themes	Concepts (vocabulary)	Student quotes	
	Theme 3(a)			
14	concentrations don't change over time		<ul> <li>E1: "I kinda realize, after seeing the graph, the reactants aren' going to be the same at equilibrium, so K very might well equal 1, not because products, mean concentration of products and reactants may not be the same, it's just K expression is equal to 1"</li> <li>E14: "I remember it talking about th concentration</li> </ul>	
			concentration staying constant when it reaches equilibrium No I think that's constant, not equal"	
			E13: "Well, again the program clearly showed, like the pulley system, it showed how if you add th weight, the ratio i constant, it's a constant thing, whenever it reaches equilibrium"	
	Question 4: At equilibrium, in terms of rate	$^{2}(N-15)$	equinorium	
N	Sub Themes	Concepts	Student quotes	
		(vocabulary)		

15	Forward and reverse reaction continue to	E3: "I mean, once
13	occur, rates are equal and constant over time	its done, its
1	occur, raies are equal and constant over time	
		basically gonna be
		levelled out, that's
		what, I get it now,
		when it meant by
		constant over time,
		that's why I decide
		to with (c), this
		time around"
		EQ. "Imm I
		E8: "Umm, I
		didn't really
		understand the
		concept of rate, I
		mean equilibrium
		rate at first, I kinda
		thought, I actually
		mixed up
		concentration and
		rate. Now I
		understand now, at
		equilibrium, in
		order for it to be at
		equilibrium, the
		rates must be equal
		and then"
		E14: "because, the
		forward and
		reverse reactions
		according to the
		graph, it showed it
		equaled out over
		time"
		<b>E13:</b> "I
		remembered
		through the
		program that
		forward and
		reverse reactions
		continue to occur
		even after
1		equilibrium is
		reached and
L		

	Ouestion 5: At equilibrium in terms of stoichi	$ometry^2 (N-15)$	forward and reverse rates are equal. Is that right, I don't know if it's right. Forward and reverse rate are constant over time, cuz the bars did not change. That's why"
	Question 5: At equilibrium, in terms of stoichi		Q. 1
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 5(a)		
3	Equal amount of NO and NOCl		E10: "Choice (b), it made the most sense"
	Theme 5(b)		

2	Equilibrium shifts toward right, hence more	E3: "I have been
	NOCl will be present	questioning A and
		B also, and I
		know, its like,
		since, NO and
		NOCl do exist in 2
		to 2 ratio, I think
		they are trying to
		be equal, but they
		never will be, its
		like close but not
		there, I could have
		chosen B, but
		couldn't have
		chosen it"

	Theme 3 – Equilit	orium Constant		
	<b>Question 6:</b> At equilibrium, what is true about equilibrium constant?(N=15)			
N	Sub Themes	Concepts (vocabulary)	Student quotes	
	Theme 6(a)			
7	Equilibrium constant (K) is less than 1			
	Theme 6(b)			
1	Equilibrium constant (K) is equal to 1, concentration of reactants and products are equal Theme 6(c)			
3	Equilibrium constant $K = 1$ , because forward and reverse rates are equal			
	Question 8: After addition of [NO], when new	v equilibrium is re-es	tablished? (N=15)	
N	Sub Themes	Concepts (vocabulary)	Student quotes	
	Theme 8(a)			
6	Equilibrium constant greater than 1	Le Chatelier's principle, arithmetic and algorithmic,	<ul> <li>E3: "After addition of NO, when equilibrium is established, constant will continue to increase"</li> <li>E5: "the pre-test I totally guessed, let me be honest. When you add NO, you gonna end with more products"</li> </ul>	
			<b>E15:</b> "If NO is added, it's going to shift to the right, both products and reactants will increase, so greater concentration of everything, and a greater K"	
	Theme 8(b)			
8	Equilibrium constant is the same			

Theme 4 – Changing equilibrium conditions		
Question 7: At equilibrium concentration of [NO] is instantaneously increased at		
constant volume (N=15)		
N Sub Themes	Concepts (vocabulary)	Student quotes
Theme 7(a)		
	slv	E1:
7 Rate of forward reaction will instantaneou increase	sly	E1:"Concentration of NO is instantaneously increased, the 

			during the
			change"
			change
			E10: "I guess like when you add the reactant, concentration of NOCl goes higher, goes up, so that's why I decide to go with (b)" E11: "I guess, whenever you initially make the change, only the forward reaction rate is changing, that's why"
			that S wily
	Theme 7(b)		
5	Rate of reverse reaction will decrease and		
	forward rate will instantaneously increase		
	Theme 7(c)		
3	Rate of reverse reaction will increase, because		E15: "Once
C	more NOCl is formed		they add the
			extra NO, the
			rate of the
			forward
			reaction
			increased
			immediately,
			and then
			became
			decreasing, so
			I was just sure
			if it meant like
			continue to
			increase, that's
			why"
	Question 9: Equilibrium is disturbed by decreas	sing the volume at const	
	temperature, initially? (N=15)	ing the volume at coms	
1	temperature, mitury. (11-13)		

N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 9(a)	(vocuoului y)	
4	Rates of forward reaction increase, reverse reaction decrease		<b>E9:</b> "Okay, Ummm, I might not have done that in that sense, but if that's not the case, I would stay with (d)"
	Theme 9(b)		
7	Rate of forward reaction increase		E2: "As soon as the volume is decreased, rate of forward reaction will increase, Ummm, basically when chemical reactions is happening, when there is less volume, there is less space for them to run around, so, they interact with each other, Ummm, so, rate of forward reaction increasing, that wouldn't cause the rate of the reverse reaction to decrease"E12: "I 
			it, I thought, one of them

			should increase and one of them should decrease, but I didn't know which one to choose, so I just went with a"
	Theme 9(c)		
1	Rate of reverse reaction increase		
	Theme 9(d)		
1	Forward reaction rate will be greater than		
	reverse reaction rate		
	Theme 9(e)		
2	Rate of forward and reverse reaction increase		<b>E1:</b> "So we
			look at the rate of the forward reaction is going to increase, because you decrease volume, the rate of the reverse reaction will also increase, so overall the reaction rate is going to increase"
	Question 10: Equilibrium is disturbed by decrea	0	istant
	temperature, when new equilibrium is re-establi		
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 10(a)		
13	Rate of forward and reverse reaction are equal and greater than the first equilibrium		E1: "Okay when new equilibrium is re-established after decreasing the volume, which

	l .	
		means you
		increase the
		pressure, rates
		of forward and
		reverse
		reaction will be
		greater than
		before, so,"
		E7: "I realized
		that rates of
		forward and
		reverse rates
		should be
		equal, but then
		also when you
		constrain the
		volume, the
		rates gonna be
		higher"
		E8:
		"Whenever the
		volume is
		decreased, it's
		gonna be
		higher
		concentration,
		so, both the
		rates are going
		to increase, in
		order for
		equilibrium to
		form again"
		<b>E14:</b> "Again,
		just comparing
		it to the visual
		and as volume
		went down,
		both rates were
		equal, but also
		greater than
		before"
ne 10(b)		

1	Rate of forward and reverse reaction will be greater in the newer equilibrium		E3: "Well now that I look at it, it is equal, I must have missed it. I guess I didn't
			interpret the graphs right or fully interpret it"
	Theme 10(c)		
1	Rate of reverse reaction increases		
	Question 11: Equilibrium is disturbed by decrea	asing the volume at co	onstant
	temperature, when new equilibrium is re-establi	shed (concentration)	(N=15)
Ν	Sub Themes	Concepts	Student quotes
		(vocabulary)	
	Theme 11(a)		
4	Concentration of NO and Cl2 will be less and		
	NOCl will be greater in the newer equilibrium		
	Theme 11(b)		
9	Concentration of NO, Cl2 and NOCl will be		<b>E2:</b> "Ummm,
	greater in the newer equilibrium		there is, the,
			the, since its at
			equilibrium,
			ratio of
			products and
			reactants is
			going to be the same. Now
			that the volume
			is lower,
			Ummm, you know,
			concentration
			is measured in
			moles per liter,
			so more moles
			less volume,
			means
			concentration
			will be higher
			than the first
			equilibrium"
			<b>E8:</b> "Well the
			simulation

			explained
			concentration
			well, well
			concentration
			is moles over
			liters, so if
			smaller
			volume,
			concentrations
			going to be
			higher for all, I
			mean reactants
			and products"
			min Pronnens
			<b>E9:</b> "The
			concentration
			graph when
			you decrease
			the volume
			was helpful.
			When you
			decrease the
			volume, you
			are increasing
			the
			concentration,
			of all of em,
			because its
			moles over
			volume"
			volume
		.	<b>E14:</b> "I
			remembered,
			cuz moles over
			volume,
			volume, volume
			decrease
			concentration
			went up"
	Theme 11(c)		
2	Concentration of NO, NOCl will be greater		<b>E11:</b> "I am just
	and Cl2 will be less in the newer equilibrium		trying to
	and C12 will be less in the newer equilibrium		remember
1			what the
			graphs looked
			graphs looked

and then the NOCl the last"				like. NO increased the most, Cl increased the second most, and then the NOCl the last"
-----------------------------	--	--	--	--

# Dissertation Study control group\_PRE-TEST

Larger theme – Conceptual Understanding

\*Participants who answered none of the above or insufficient information provided are not included for analysis in the table, as they do not constitute a theme. In some cases none of the above or insufficient information is the correct answer\*

	Theme1 – Approach	ing Equilibrium	
	<b>Question 1:</b> As the reaction approaches equilibrium		? (N=15)
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 1(a)	()	
1	Rate of forward and reverse rate decreases at		
	the same rate		
	Theme 1(b)		
3	The rate of the forward reaction decreases		
	Theme 1 (c)		
5	Reverse and forward rates are equal		C3: "you know, at equilibrium, rates of forward and reverse are equal, so I decide to go with E" C4: "I mean when it's getting close to equilibrium, they are starting to become, the rate at which the forward and reverse reactions
	Theme 1 (d)		become equal"
2	Rate of forward reaction increases		
	<b>Question 2:</b> As the reaction approaches equilibrium	rium in terms of con	$\frac{ }{(N-15)}$
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 2(a)		
4	Concentration of reactants and products is constant, because K <1		
3	Theme 2(b) Concentration of reactants and products is equal		C2: "Oh the reaction when it's at

		equilibrium, the reactants and products concentration are equal"
	Theme 2(c)	
3	Concentration of reactants is 3 times more than concentration of products	

	Theme 2 – Characteristics of Equilibrium				
	<b>Question 3:</b> At equilibrium, in terms of concentration? (N=15)				
N	Sub Themes	Concepts (vocabulary)	Student quotes		
	Theme 3(a)				
4	Concentration of reactants and products is equal because equilibrium constant K=1		<ul> <li>C4: "Well, equilibrium means K =1"</li> <li>C10: "I choose A because K =1, its equal, so equilibrium"</li> <li>C11: "I thought of equilibrium, so K must be equal to 1, and hence concentrations must be equal"</li> </ul>		
	Theme 3(b)				
5	concentrations don't change over time		<ul> <li>C1: "I remember, I remember, while learning, when you had equilibrium, I just remembered concentration of reactants and products are constant because, the rates were staying the same"</li> <li>C9: "I said C because, neither A or B is correct"</li> </ul>		
	Theme 3(c)				

2	Concentration of reactants and products is greater, because K>1		<ul> <li>C6: "there is less moles of products and more moles of reactants, so I decide to go with K less than 1, which is B"</li> <li>C5: "because there is more moles of products, so if I put it in the equilibrium expression, K must be less than 1"</li> </ul>
	Question 4: At equilibrium, in terms of rat	e? (N=15)	
Ν	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 4(a)		
1	Forward and reverse reaction continue to occur		
	Theme 4(b)		
5	Forward and reverse rates are equal Theme 4(c)		
6	Forward and reverse reaction continue to occur, rates are equal and constant over time		
	Question 5: At equilibrium, in terms of sto	ichiometry? (N=15)	
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 5(a)		

6	Equal amount of NO and NOCl	C1: "so they do have a 2 to 2 stoichiometry, I knew that at equilibrium, C wasn't going to be right, as it doesn't shift, I don't think Cl2 is going to be a limiting reagent, cuz its at equilibrium, I thought B sounded right, as we did ICE table, I remembered using coefficients" C2: "Since it's a 2 to 2
		ratio, it makes sense, the amounts go to be equal. So that's why I decide to go with B"
		<b>C5:</b> "both NO and NOCl got coefficients of 2, so when equilibrium is attained, they should both be in equal amounts"
		<b>C12:</b> "I didn't know if it's A or B, because Cl2 is less, so it could be limiting, but I decide to go with B, it's the strongest of the two"
	Theme 5(b)	
1	Equilibrium shifts toward right, hence more NOCl will be present	
	Theme 5(c)	
3	Cl2 is the limiting reagent, no Cl2 will be left	<b>C9:</b> "because, in the equilibrium equation given, Cl2 was the limiting reagent"

	Theme 3 – Equilibrium Constant		
	<b>Question 6:</b> At equilibrium, what is true about equilibrium constant?(N=15)		
Ν	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 6(a)		
4	Equilibrium constant (K) is less than 1		C1: "I kinda forgot what K was, a little bit, I do remember it was products over reactants, and I knew that it would be NOCI squared over NO squared and Cl2. I kind guessed it to be less than 1, I just wasn't sure there either. I guessed products will be less than reactants"
	Theme 6(b)		
1	Equilibrium constant (K) is greater than 1		
	Theme 6(c)		
1	Equilibrium constant (K) is equal to 1, concentration of reactants and products are equal		C2: "As I am not sure about the K thing. But reading everything D made the most sense"
	Theme 6(d)		
4	Equilibrium constant K =1, because forward and reverse rates are equal		C4: K =1 is right, so I decide to go with D.
	Question 8: After addition of [NO], when new equil	ibrium is re-established? (	N=15)
Ν	Sub Themes	Concepts (vocabulary)	Student quotes

	Theme 8(a)	
3	Equilibrium constant greater than 1	C8: "I choose B, addition of NO will make the constant greater"C10: "I decide to go with B, because when you add NO, the equilibrium will shift to right, so you'll have more of NOCl, so
		according to the K expression, K will be greater"
	Theme 8(b)	
6	Equilibrium constant is the same	C5: "I decide to go with A for #8, was, because, addition of NO is offset with the heat"

	Theme 4 – Changing equilibrium conditions			
	Question 7: At equilibrium concentration of [NO] is instantaneously increased at constant			
	volume (N=15)		-	
Ν	Sub Themes	Concepts	Student quotes	
		(vocabulary)		
	Theme 7(a)			
2	Rate of forward reaction will			
	instantaneously increase			
	Theme 7(b)			
1	Rate of forward reaction will			
	not change, as volume is kept			
	constant			
	Theme 7(c)			
3	Rate of forward reaction			
	increase, reverse reaction			
	decrease			
	Theme 7(d)			
5	Rate of reverse reaction will			
	increase, because more NOCl is			
	formed			
	Theme 7(e)			
1	Rate of forward reaction and			
	reverse reaction will increase			
		bed by decreasi	ng the volume at constant temperature,	
	initially? (N=15)	1		
Ν	Sub Themes	Concepts	Student quotes	
		(vocabulary)		
	Theme 9(a)			
4	Rates of forward reaction		C1: "I know when volume decreases	
	increase, reverse reaction		pressure decreases, and there is 3moles	
	decrease		on the reactant side and 2 moles on the	
			product side and its gonna wanna go to	
			the side with less moles, so I knew that	
			the forward reaction was going to	
			increase and the reverse reaction was	
			going to decrease, so I picked C"	
	Theme 9(b)			
2	Rate of forward reaction			
	increase			
	Theme 9(c)			
3	Rate of reverse reaction			
	decrease			
1	Theme 9(d)			

1	Forward reaction rate will be		
	greater than reverse reaction		
	rate		
	Theme 9(e)		
2	Rate of reverse reaction increase		
-	Question 10: Equilibrium is distu	irbed by decreas	ing the volume at constant temperature,
	when new equilibrium is re-estable	lished (rate) (N	=15)
Ν	Sub Themes	Concepts	Student quotes
		(vocabulary)	
	Theme 10(a)		
3	Rate of forward reaction		
	increase and		
	Rate of reverse reaction		
	decreases		
	Theme 10(b)		
3	Rate of forward reaction		
	increase		
	Theme 10(c)		
4	Rate of reverse reaction increase		
	Theme 10(d)		
2	Rate of reverse reaction		<b>C10:</b> "I put B, because the volume is
	decreases		decreased, the equilibrium should shift
			right, and so reverse reaction would
			slow down, so I went with B"
			<b>C7</b> : "decreasing the volume and the rate
			of the reaction would decrease"
			ing the volume at constant temperature,
	when new equilibrium is re-estable		
Ν	Sub Themes	Concepts	Student quotes
		(vocabulary)	
_	Theme 11(a)		
5	Concentration of NO and Cl2		C1: "Decrease volume means increase
	will be less and NOCl will be		pressure, 3 moles on the reactant side
	greater in the newer equilibrium		and 2 moles on the product side, it's
			gonna shift to the side with less moles,
			and I know that the reaction is going to
			shift to the right, to decrease the
			pressure, the NO and Cl2 would
			decrease and NOCl would increase"
			C2. "Wall if you doggood the walvest
			<b>C3:</b> "Well if you decrease the volume,
			you go towards the side with less
1		1	amount of gas, and that was on the right

		<ul> <li>side. So equilibrium will shift towards right, and I selected choices that fitted the logic. That's how I ended up with a, d &amp; e"</li> <li>C4: "I wasn't entirely sure, I just went off with the strongest choice possible, I used Le Chatelier's principle to make my decision"</li> </ul>
2	Theme 11(b) Concentration of NO, Cl2 and NOCl will be greater in the newer equilibrium Theme 11(c)	
1	Concentration of NO will be less Theme 11(d)	C5: "because volume was decreased, so that would lower the products"
1	Concentration of NO will be greater	<b>C6:</b> "I went with increased pattern for the whole test"
1	Theme 11(e) Concentration of Cl2 will be less	<b>C10:</b> "I picked D, because when I read decreasing volume, I went with a choice that was decreasing"
2	Theme 11(f) Concentration of NOCl will be greater	<ul> <li>C7: "I picked E, because, with the reaction, there is not enough of it to keep the reaction going, so concentration of NOCl will be greater"</li> <li>C12: "It was a process of elimination, since A and B did not appear to be true, I eliminated choices containing A and B, and the since we decrease volume, there will be more products, so I decide to go with E"</li> </ul>

#### Dissertation Study control group\_POST-TEST

Larger theme – Conceptual Understanding

\*Participants who answered none of the above or insufficient information provided are not included for analysis in the table, as they do not constitute a theme. In some cases none of the above or insufficient information is the correct answer\*

	Theme1 – Approach	ing Equilibrium	
	Question 1: As the reaction approaches equilib	prium, in terms of rate? (N	I=15)
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 1(a)		
4	Rate of forward and reverse rate increase at the same rate		C4: "Due to the fact, its approaching and not at equilibrium, that's why I decide to change my answer"
	Theme 1(b)		
2	The rate of the forward reaction decreases		
	Theme 1 (c)		
5	Reverse and forward rates are equal		
	Question 2: As the reaction approaches equilib	orium, in terms of concent	ration? (N=15)
N	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 2(a)		
5	Concentration of reactants and products is constant, because K <1		
	Theme 2(b)		
2	Concentration of reactants and products is equal		
	Theme 2(c)		
2	Concentration of reactants is 3 times more than concentration of products		

	Theme 2 – Characteristics of Equilibrium										
	<b>Question 3:</b> At equilibrium, in terr										
	Sub Themes	Concepts (vocabulary)	Student quotes								
	Theme 3(a)	Concepts (vocuoulary)	Student quotes								
4	Concentration of reactants and products is equal because equilibrium constant K=1		<ul> <li>C4: "I choose, A because, because of, at equilibrium, they have to be equal, as from the notes, I got the idea K is equal to 1"</li> <li>C10: "but this time around I put a little more logic in it, I just went with A"</li> <li>C8: "I forgot what exactly my logic was. I choose A</li> </ul>								
			this time"								
	Theme 3(b)										
	concentrations don't change over										
	time										
	Theme 3(c)										
2	Concentration of reactants and										
	products is greater, because K>1										
NT	Question 4: At equilibrium, in terr										
	Sub Themes	Concepts (vocabulary)	Student quotes								
	Theme 4(a)										
	Forward and reverse reaction										
	continue to occur Thoma 4(b)										
	Theme 4(b) Forward and reverse rates are										
	equal										
	Theme 4(c)										
1	Forward and reverse reaction										
	rates are equal and constant over										
	time										
	Theme 4(d)										
	Reverse rate is greater than										
	forward rate										
	Theme 4(e)										
	Forward and reverse reactions										
	continue to occur, rates are equal										
	and constant										

	Theme 4(f)		
1	Reactions continue to occur and		
	rate is constant over time		
	Question 5: At equilibrium, in terr	ns of stoichiometry? (N=1	15)
Ν	Sub Themes	Concepts (vocabulary)	Student quotes
	Theme 5(a)		
9	Equal amount of NO and NOCl		
	Theme 5(b)		
2	Cl2 is the limiting reagent, no		
	Cl2 will be left		

	Theme 3 – Equilibrium Constant								
	<b>Question 6:</b> At equilibrium, what is	true about equilib	orium constant?(N=15)						
Ν	Sub Themes	Concepts	Student quotes						
	Theme 6(a)	(vocabulary)							
5	Equilibrium constant (K) is less								
	than 1								
	Theme 6(b)								
3	Equilibrium constant (K) is equal								
	to 1, concentration of reactants and								
	products are equal								
	Theme 6(c)								
3	Equilibrium constant K =1,								
	because forward and reverse rates								
	are equal								
	<b>Question 8:</b> After addition of [NO], when new equilibrium is re-established? (N=15)								
N	Sub Themes	Concepts	Student quotes						
		(vocabulary)							
	Theme 8(a)								
	Equilibrium constant greater than 1								
	Theme 8(b)								
	Equilibrium constant is the same								

	Theme 4 – Chang	ing equilibrium condi	tions
	<b>Question 7:</b> At equilibrium concent		
	at constant volume (N=15)		•
N	Sub Themes	Concepts	Student quotes
		(vocabulary)	-
	Theme 7(a)	•	
4	Rate of forward reaction will		
	instantaneously increase		
	Theme 7(b)		
2	Rate of forward reaction will not		
	change, as volume is kept constant		
	Theme 7(c)		
3	Rate of forward reaction increase,		
	reverse reaction decrease		
	Theme 7(d)		
2	Rate of reverse reaction will		
	increase, because more NOCl is		
	formed		
	Theme 7(e)		
1	Rate of reverse reaction will		
	decrease		
	<b>Question 9:</b> Equilibrium is disturbe	d by decreasing the vol	ume at constant
	temperature, initially? (N=15)	, ,	
N	Sub Themes	Concepts	Student quotes
		(vocabulary)	1
	Theme 9(a)	, , , , , , , , , , , , , , , , , , ,	
5	Rates of forward reaction increase,		
	reverse reaction decrease		
	Theme 9(b)		
3	Rate of forward reaction increase		
	Theme 9(c)		
	Rate of reverse reaction decrease		
1	Theme 9(d)		
1	Forward reaction rate will be		
	greater than reverse reaction rate		
	Theme 9(e)		
1	Rate of reverse reaction increase		
1	<b>Question 10:</b> Equilibrium is disturb	ed by decreasing the vo	olume at constant
	temperature, when new equilibrium		
N	Sub Themes	Concepts	Student quotes
		(vocabulary)	Student quotes
	Theme 10(a)	( · · · · · · · · · · · · · · · · · · ·	
1	Rate of forward reaction increase		
•	and		
	Rate of reverse reaction decreases		
	Theme 10(b)		
2	Rate of forward and reverse		
-	reaction greater in the newer		
	reaction greater in the newer		

	Theme 10(c)		
7	Rate of reverse reaction increase		
	Theme 10(d)		
2	Rate of reverse reaction decreases		
	Question 11: Equilibrium is disturbed	ed by decreasing the vo	lume at constant
	temperature, when new equilibrium	is re-established (conce	ntration) (N=15)
Ν	Sub Themes	Concepts	Student quotes
		(vocabulary)	
	Theme 11(a)		
10	Concentration of NO and Cl2 will		
	be less and NOCl will be greater in		
	the newer equilibrium		
	Theme 11(b)		
2	Concentration of NO and NOCl		
	will be greater and Cl2 will be less		
	in the newer equilibrium		

# **APPENDIX D**

### CODING FOR CONDITIONAL PROBABILITY ANALYSIS

a CA-CR	Item	Reasoning	# of students	Item	Reasoning	# of students	Item	Reasoning	# of students
b CA-IR	1	1a	2	5	5a	3	9	9a	1
c IA-IR		1b			5b			9b	
d IA-CR		1c	10		5c	12		9c	14
e CA-NR		1d			5d			9d	
		1e	3		5e			9e	
	2	2a	6	6	ба		10	10a	
		2b			6b			10b	
		2c	7		6c	13		10c	1
		2d			6d			10d	
		2e	2		6e	2		10e	
	3	3a	6	7	<b>7</b> a	1	11	11a	
		3b			7b			11b	
		3c	6		7c	14		11c	1
		3d			7d			11d	
		3e	3		7e			11e	
	4	4a	1	8	8a	3			
		4b			8b				
		4c	7		8c	5			
		4d			8d				
		4e	7		8e	7			

Figure 21: Matrix representing the number of students assigned to a condition for each item based on the pre-test data for the experimental group

a CA-CR	Item	Reasoning	# of students	Item	Reasoning	# of students	Item	Reasoning	# of students
b CA-IR	1	1a	5	5	5a	6	9	9a	4
c IA-IR		1b			5b			9b	
d IA-CR		1c	1		5c	5		9c	8
e CA-NR		1d			5d			9d	
		1e	9		5e	4		9e	3
	2	2a	6	6	ба	2	10	10a	6
		2b			6b			10b	
		2c	5		6c	12		10c	2
		2d			6d			10d	
		2e	4		6e	1		10e	7
	3	3a	6	7	7a	5	11	11a	6
		3b			7b			11b	
		3c	1		7c	8		11c	6
		3d			7d			11d	
		3e	8		7e	2		11e	3
	4	4a	8	8	8a	3			
		4b			8b				
		4c	0		8c	7			
		4d			8d				
		4e	7		8e	5			

Figure 22: Matrix representing the number of students assigned to a condition for each item based on the post-test data for the experimental group

# of students	Reasoning	Item	# of students	Reasoning	Item	# of students	Reasoning	Item	a CA-CR
1	9a	9	1	5a	5	1	1a	1	b CA-IR
	9b			5b			1b		c IA-IR
10	9c		10	5c		9	1c		d IA-CR
	9d			5d			1d		e CA-NR
1	9e		2	5e		2	1e		
(	10a	10	1	ба	6	2	2a	2	
	10b			6b			2b		
12	10c		8	6c		10	2c		
	10d			6d			2d		
	10e		3	6e			2e		
	11a	11		7a	7	1	3a	3	
1	11b			7b			3b		
10	11c		10	7c		9	3c		
	11d			7d			3d		
1	11e		2	7e		2	3e		
			2	8a	8		4a	4	
				8b			4b		
			6	8c		6	4c		
				8d			4d		
			4	8e		6	4e		

Figure 23: Matrix representing the number of students assigned to a condition for each item based on the pre-test data for the control group

a CA-CR	Item	Reasoning	# of students	Item	Reasoning	# of students	Item	Reasoning	# of students
b CA-IR	1	1a	2	5	5a	1	9	9a	3
c IA-IR		1b			5b			9b	
d IA-CR		1c	10		5c	11		9c	9
e CA-NR		1d			5d			9d	
		1e			5e			9e	
	2	2a	3	6	ба	1	10	10a	0
		2b			6b			10b	
		2c	9		6c	9		10c	12
		2d			6d			10d	
		2e			6e	2		10e	
	3	3a	1	7	7a	1	11	11a	2
		3b			7b			11b	
		3c	9		7c	8		11c	10
		3d			7d			11d	
		3e	2		7e	3		11e	
	4	4a	2	8	8a	2			
		4b			8b	1			
		4c	7		8c	8			
		4d			8d				
		4e	3		8e	1			

Figure 24: Matrix representing the number of students assigned to a condition for each item based on the post-test data for the control group

## **APPENDIX E**

### SAMPLE INTERVIEW TRANSCRIPT

R: Researcher

P: Participant

\_\_\_\_\_

1D2C (PRE)

R: Okay for #3, This is the reaction has its shown here, you choice (a) right? Why, why did you choose choice (a)?

P: The concentration of reactants and products equal if K=1 that's what it reads, so when by definition K is equal to 1, when the concentration of products and reactants is the same, well, it's the same, yeah, it's the same, cuz it's products over reactants and so when you divide the top by the bottom, you get 1, so K equals to products over reactants

R: very good, good

R: For #2, you choose none of the above right, so what was your reasoning behind why you chose (e)?

P: When you look through a through d, first one reads concentration of reactants and products is equal because K is equal to 1, this is, we are not at equilibrium, so K can't be equal to 1, so for (b) concentration of reactants is 3 times more than products. If you have 3 times more reactants, K must be less than 1. Concentration of reactants is 3 times less than products, well, Uhh, you would have, K is equal to 3 times whatever it was. Concentration of reactants and products isn't constant cuz we are approaching equilibrium.

R: Okay for #5, you choose (b) right, so what there a particular reason why decide to go with (b)?

P: Cuz, NO and NOCl exists in a 2 to 2 stoichiometry, there will be equal amount of NO and NOCl, stoichiometrically we say that for every amount of NO, we have at a same constant ratio the amount that's on the right which is NOCl

R: So why can't it be (c)?

P: (c) reads equilibrium shifts to the right, hence more NOCl will be present, well at equilibrium, and there is no shifting, because you are not adding or subtracting anything, which is why

R: For #7, it reads the system is already at equilibrium and you disturb it by adding more NO, right? and you decide to go with choice (e) what was your reasoning behind why you choose (e)?

P: Well, when you add, by le Chatelier's principle, you have to shift to the side that relieves the stress, I said the rate of the reverse reaction will decrease because, equilibrium shifts towards the right, so that's pretty explanatory, the rate of the forward reaction will increase

R: Can you draw or show mathematically, like, tell me how you feel, how you see rate of forward reaction is increasing? How do you see that? The process?

P: I see, when I think of, Okay, you got few molecules here and when you try to infuse it with more and more molecules, you have a constant rate right here, but when you pitching more and more, you got even higher rate.

R: So when it says increases, I mean, how do we define rate? I mean what is rate?

P: Rate is the amount of, the products that's being reduced in a certain amount of time.

R: Okay, amount of products being or reactants being reduced?

P: Yeah, products being reduced

R: is it for the forward reaction?

P: Yeah, it is for the forward reaction

R: Okay for #9, you decide to go with choice c, which is a & b, why is that?

P: Ummm, [long pause], well I had to think about this one

R: No problem, take your time

P: Well, you decrease volume, so you increase pressure, so it will move to right, so reaction cannot move to left, so, it's like, the, the forward should increase and reverse should decrease

R: You mean the rate?

P: Yeah that's what I meant

R: Thanks

R: okay, let's go with #11, the system is at equilibrium right? And you disturb it by decreasing volume, equilibrium has to re-establish right? Cuz all reversible reactions eventually has to get back to equilibrium right? So why you choose a, d and e?

P: okay (a) reads concentration of NO will be less than the first equilibrium. Okay when we take away volume, we got lot of this NO and Cl2, actually you got 2 NO's and one Cl2, these take up more space collectively than NOCl would, so if we decrease the volume, in order to relieve the most amount of stress on the system, we have to take away, we want to put, we want to have the same amount of products. So you go to the side with the least amount of stress, so we go to right, going to (d), we have the concentration of Cl2 will be less than first, and the concentration of NOCl would have to increase as in (e).

1D2C (POST)

R: Okay for #3, you may have changed your answer, that does not mean it's right or wrong? For # 3 you choose (a), on your post-test you decide to go with (c), why is that?

P: I kinda realize, after seeing the graph, the reactants aren't going to be the same at equilibrium, so K very might well equal 1, not because products, I mean concentration of products and reactants may not be the same, its just K expression is equal to 1, because its

R: So why do we say K equals 1. I mean, I really understood your logic, If in algebra we say, the ratio equals 1, what do we assume?

P: Well, if you assume, your ratio is 1, you have the same amount on one side and the same on the opposite side.

R: So if we say its constant as in (c), right, but we say equilibrium means K equals 1, what are we really refer to, these two cannot be equal, than how can K be equal to 1?

P: I would say the ratio of going from one end to the other is the same

R: so what is that ratio called?it's called by a different name.

P: May be rate?

R: Okay #5, you indicated a (b) on your pre-test, this time you decide to go with (d) why is that?

P: Again, because NO and NOCl exists in a 2 to 2 stoichiometry, there won't be equal amounts of NO and NOCl. I think the visual part of the thing, it was, it is, it really helped me to understand what the concentrations would be. Concentrations of NO, Cl2 and NOCl did not go to one thing, it were, it was, you know, NO was its one thing, Cl2 was its one thing

R: Okay, will it ever be the same? Under any circumstances would it ever be the same? Can we say that? If it's not equal, what makes it that way?

P: Because equilibrium is dynamic, when you change one thing, in this case if you change NO, you change two others, so I think that's probably why

R: For your pre-test for #7, you decide to go with a, this time you decide to go with (b), why is that?

P: Concentration of NO is instantaneously increased, the reverse reaction will in fact increase, when you suddenly increase the amount of NO, there is going to be a huge surge of NOCl being created, and to compensate for that increase

R: so you said a surge of NOCl being created, and so what do we mean by the rate of the forward reaction increased? What are we really referring to? What is increasing in terms of the rate?

P: As you increase the amount of NO, suddenly, you are going to have a certain amount of increase in NOCl, to compensate for the increase in NO,

R: Okay, let me ask you this, what does rate refers to?

P: It's referring to change in the amount, I mean the molarity with change of time

R: Okay, in this context when you say rate of forward reaction will increase, what are we referring to?

P: We are referring to, the total amount of NOCl created over time,

R: Okay for #9, I think on your pre-test, you indicated choice (c), for your post-test you indicated a & d what was the reasoning?

P: So we look at the rate of the forward reaction is going to increase, because you decrease volume, the rate of the reverse reaction will also increase, so overall the reaction rate is going to increase

R: so did you read the question says initially, right when a change is made

P: [laughs], no I didn't

R: For #10, you indicated (c) as your choice, this time you decide to go with (f), what was your reasoning behind the change?

P: Okay when new equilibrium is re-established after decreasing the volume, which means you increase the pressure, rates of forward and reverse reaction will be greater than before, so,

R: Why do you think its greater?

P: Rate = k\*times.

P: I don't think that's right,

R: No go ahead and complete it, this is one way of writing it

R: So how did we define rate earlier in our interview?

P: We said concentration over time

R: Why do you think rate is greater, what made rate greater?

P: more stress on reactants and products, to compensate, subsequent increase in NOCl, there is also going on in the reverse direction,

R: So what is increased in the ratio?

P: The concentration of the products and the reactants?

R: Very good, good

R: Last time for #11 a, d and e, this time you have b, d and e, why was that?

P: so we see, when new equilibrium is re-established, Concentration of NO will be greater in the new equilibrium

R: Why is that?

P: Concentration is a measure of number of moles per volume

P: When you decrease volume, you decrease the denominator, that's why increase in concentration, Concentration of NOCl will be greater, there will be more products according to Le Chatelier's principle.

R: Well thanks for your support, I sincerely appreciate it

P: You're welcome, good luck with the study

## **APPENDIX F**

### **INSTITUTIONAL REVIEW BOARD (IRB) – APPROVAL LETTER**

. 9	IK		
	KENTUCKY	7°	
		Lit	
			Office of Research Integrity IRB, IACUC, RDRC 315 Kinkead Hall Lexington, KY 40506-0057
	Continuation Expedited Review		859 257-9428 fax 859 257-8995
Procedures; Meas	roved: Extension; Research Description; ures; Consent		www.research.uky.edu/ori/
Approval Ends December 5, 2010	S CN DISS	IRB Number 14-0897-P4S	
то:	Bharath Kumar 1320 Versailles Road Apt. 8 Lexington, KY 40504 PI phone #: (859)705-5250		
FROM:	Chairperson/Vice Chairperson Non-medical Institutional Review Board (IRB)	the next extransion	and the second
SUBJECT:	Approval of Protocol Number 14-0897-P4S		
DATE:	December 10, 2015		

Evaluating the role of instructional technology towards students' conceptual understanding of chemical equilibrium

Approval is effective from December 7, 2015 until December 5, 2016 and extends to any consent/assent form, cover letter, and/or phone script. If applicable, attached is the IRB approved consent/assent document(s) to be used when enrolling subjects. [Note, subjects can only be enrolled using consent/assent forms which have a valid "IRB Approval" stamp unless special waiver has been obtained from the IRB.] Prior to the end of this period, you will be sent a Continuation Review Report Form which must be completed and returned to the Office of Research Integrity so that the protocol can be reviewed and approved for the next period.

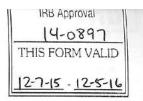
In implementing the research activities, you are responsible for complying with IRB decisions, conditions and requirements. The research procedures should be implemented as approved in the IRB protocol. It is the principal investigator's responsibility to ensure any changes planned for the research are submitted for review and approval by the IRB prior to implementation. Protocol changes made without prior IRB approval to eliminate apparent hazards to the subject(s) should be reported in writing immediately to the IRB. Furthermore, discontinuing a study or completion of a study is considered a change in the protocol's status and therefore the IRB should be promptly notified in writing.

For information describing investigator responsibilities after obtaining IRB approval, download and read the document "PI Guidance to Responsibilities, Qualifications, Records and Documentation of Human Subjects Research" from the Office of Research Integrity's IRB Survival Handbook web page [http://www.research.uky.edu/ori/IRB-Survival-Handbook.html#Plresponsibilities]. Additional information regarding IRB review, federal regulations, and institutional policies may be found through ORI's web site [http://www.research.uky.edu/ori]. If you have questions, need additional information, or would like a paper copy of the above mentioned document, contact the Office of Research Integrity at (859) 257-9428.

Chairperson/Vice Chairperson

## APPENDIX G

### **INSTITUTIONAL REVIEW BOARD (IRB) – CONSENT FORM**



#### Consent to Participate in a Research Study

## EVALUATING THE ROLE OF INSTRUCTIONAL TECHNOLOGY TOWARDS STUDENTS' CONCEPTUAL UNDERSTANDING OF CHMICAL EQUILIBRIUM

#### WHY ARE YOU BEING INVITED TO TAKE PART IN THIS RESEARCH?

You are being invited to take part in a research study about understanding the efficiency of instructional technology towards conceptual understanding of chemical equilibrium phenomena. You are being invited to take part in this research study because the study requires students have received instruction on chemical equilibrium and related concepts. Prior knowledge of principles associated with chemical equilibrium is vital towards the study

#### WHO IS DOING THE STUDY?

The person in charge of this study is Bharath Sampath Kumar, doctoral student in the Department of STEM Education at the University of Kentucky. He is being guided in this research by *Dr. Rebecca Krall.* There may be other people on the research team assisting at different times during the study.

#### WHAT IS THE PURPOSE OF THIS STUDY?

By doing this study, we hope to learn how "instructional technology through simulations can efficiently help students' conceptually understand chemical equilibrium". The study would also open doors do conduct more study exploring the possibility of using instructional technology towards other chemistry and science concepts.

#### ARE THERE REASONS WHY YOU SHOULD NOT TAKE PART IN THIS STUDY?

If you are a minor, meaning below 18 years of age, you cannot participate in this study.

#### WHERE IS THE STUDY GOING TO TAKE PLACE AND HOW LONG WILL IT LAST?

The study will occur on University of Kentucky Main campus in Lexington, KY. As the activities contain computer simulations, the research study will take place in a computer lab. A computer lab will be reserved for the purpose of the research study. The aim is to complete the research study before the end of Fall 2016 semester.

#### WHAT WILL YOU BE ASKED TO DO?

Participants in the experimental and control groups will complete the quantitative and the qualitative portion of the study. Quantitative method involve students answering multiple choice content questions contained in a survey. The results from the quantitative method would allow us to determine participants who will be chosen for the qualitative portion of the study. For instance if 6 out of 30 students in the control group and 6 out of 30 students in the experimental group will be selected for the qualitative study. Out of the 6students, 2 students will be randomly selected from the lower end of the performance continuum, 2 students will be randomly selected from the middle end of the performance continuum and 2 students will be randomly selected from the higher end of the performance continuum on the quantitative test. Similar selection will be made among the 6 students in the

University of Kentucky Revised 9/10/14

1

F2.0150 Nonmedical IRB ICF Template

# IRB

experimental group. The chosen 6 students will be interviewed using the guiding questions listed under research procedure on Form B. Each student will be interviewed using all guiding questions for all 6 content questions in the qualitative assessment. The qualitative portion would involve audio recording of participants thought process and how they went about answering the questions, how did they arrive at such a thought or what prior knowledge had led them to such a thought etc. Students would also be asked to write or draw their thoughts. As a researcher this would allow me to look in to their thought processes.

As the first step in the research study you will be asked to read and sign a copy of the consent form. After students have signed the consent form, an electronic survey will be sent to those students to gather background information such as gender, name, email address and list of available times etc. Once available times have been received students will be contacted to schedule a time to participate in the study. Assignment of students to control or experimental groups is purely random.

Participants in the control group would only meet once during the research study. The purpose of the control group is to provide evidence if in fact only the intervention provided to the experimental group has resulted in a change. As a participant in the control group, you will first complete a quantitative survey containing a list of multiple choice questions. You will then participate in the qualitative portion where you will sit one on one with the researcher and complete an interview process. During the interview process, the researcher will be audio recording your thought processes on paper. The quantitative instrument should take approximately 30-60 minutes per person to complete. The qualitative method would last approximately 3 hours per person.

Participants in the experimental group would meet on seven different occasions. During the first meeting, they would complete the quantitative pre-test portion of the study. During the second meeting, they would sit with me for a one on one interview and complete the qualitative pre-test portion of the study. The quantitative method would last **approximately 30-60 minutes per person** to complete. The qualitative method would last **approximately 30-60 minutes per person** to complete. The qualitative pre-test portion of the study. The the intervention. During the sixth and seventh time, they will complete the post quantitative and qualitative portion of the study respectively. The total intervention time for all three occasions should last no more than 3 hours (i.e., 1 hour per session). The quantitative method would last **approximately 30-60 minutes per person** to complete. The qualitative per tensor to complete. The qualitative per tensor to use the study respectively. The total intervention time for all three occasions should last no more than 3 hours (i.e., 1 hour per session). The quantitative method would last **approximately 30-60 minutes per person** to complete. The qualitative method would last **approximately 3 hours per person**.

#### WHAT ARE THE POSSIBLE RISKS AND DISCOMFORTS?

There are no known risks are discomforts associated with the study.

#### WILL YOU BENEFIT FROM TAKING PART IN THIS STUDY?

There is no guarantee you will receive any benefit from participation in this research study.

#### DO YOU HAVE TO TAKE PART IN THE STUDY?

If you decide to take part in the study, it should be because you really want to volunteer. You will not lose any benefits or rights you would normally have if you choose not to volunteer. You can stop at any time during the study and still keep the benefits and rights you had before volunteering. As a student, if you decide not to take part in this study, your choice will have no effect on your academic status or grade in the class.

#### IF YOU DON'T WANT TO TAKE PART IN THE STUDY, ARE THERE OTHER CHOICES?

If you do not want to be in the study, there are no other choices except not to take part in the study.

#### WHAT WILL IT COST YOU TO PARTICIPATE?

There are no costs associated with taking part in the study.

#### WILL YOU RECEIVE ANY REWARDS FOR TAKING PART IN THIS STUDY?

University of Kentucky Revised 9/10/14 2

F2.0150 Nonmedical IRB ICF Template

You will receive no rewards for taking part in this study

#### WHO WILL SEE THE INFORMATION THAT YOU GIVE?

We will make every effort to keep confidential all research records that identify you to the extent allowed by law.

Your information will be combined with information from other people taking part in the study. When we write about the study to share it with other researchers, we will write about the combined information we have gathered. You will not be personally identified in these written materials. We may publish the results of this study; however, we will keep your name and other identifying information private.

Student ID, Link blue credential, telephone numbers and social security numbers will not be collected from any participants. The above mentioned items have no relevance to the purpose of the study and hence will not be obtained from participants.

We will make every effort to prevent anyone who is not on the research team from knowing that you gave us information, or what that information is. All records will be kept confidential in secured office drawers designated for this purpose. The drawer would be locked and only designated personnel on this study would have access to the study. The designated personnel's on this study would be self (principal investigator) and research advisor (Dr. Rebecca Krall). Anybody else would have no direct access to the records. Dissertation committee members would only have access to processed statistical data and would have no personal contact with participants before, during or after the study.

Only researchers will have access to all research records. However, we may be required to show information which identifies you to people who need to be sure we have done the research correctly; these would be people from such organizations as the University of Kentucky.

Please be aware, while we make every effort to safeguard your data once received from the online survey/data gathering company, given the nature of online surveys, as with anything involving the Internet, we can never guarantee the confidentiality of the data while still on the survey/data gathering company's servers, or while en route to either them or us. It is also possible the raw data collected for research purposes may be used for marketing or reporting purposes by the survey/data gathering company after the research is concluded, depending on the company's Terms of Service and Privacy policies.

#### CAN YOUR TAKING PART IN THE STUDY END EARLY?

If you decide to take part in the study you still have the right to decide at any time that you no longer want to continue. You will not be treated differently if you decide to stop taking part in the study.

The individuals conducting the study may need to withdraw you from the study. This may occur if you are not able to follow the directions they give you, if they find that your being in the study is more risk than benefit to you

#### WHAT ELSE DO YOU NEED TO KNOW?

There is a possibility that the data collected from you may be shared with other investigators in the future. If that is the case the data will not contain information that can identify you unless you give your consent or the UK Institutional Review Board (IRB) approves the research. The IRB is a committee that reviews ethical issues, according to federal, state and local regulations on research with human subjects, to make sure the study complex with these before approval of a research study is issued.

#### **Contacting Research Subjects for Future Studies**

Do you give your permission to be contacted in the future by <u>Bharath Sampath Kumar</u> regarding your willingness to participate in future research studies

Yes	No No	Initials

University of Kentucky Revised 9/10/14 3

F2.0150 Nonmedical IRB ICF Template

#### WHAT IF YOU HAVE QUESTIONS, SUGGESTIONS, CONCERNS, OR COMPLAINTS?

Before you decide whether to accept this invitation to take part in the study, please ask any questions that might come to mind now. Later, if you have questions, suggestions, concerns, or complaints about the study, you can contact the investigator, <u>Bharath Sampath Kumar</u> at <u>859-705-5250</u>. If you have any questions about your rights as a volunteer in this research, contact the staff in the Office of Research Integrity at the University of Kentucky between the business hours of 8am and 5pm EST, Mon-Fri. at 859-257-9428 or toll free at 1-866-400-9428. We will give you a signed copy of this consent form to take with you.

Signature of person agreeing to take part in the study

1

Date

Date

Printed name of person agreeing to take part in the study

Name of (authorized) person obtaining informed consent

#### REFERENCES

- AAAS (1993). Benchmarks for science literacy. Washington, DC: Author. AAAS (2001). Atlas of science literacy. Washington, DC: Author.
- Abraham, M. R., Grzybowski, E. B., Renner, J. W., & Marek, E. A. (1992). Understandings and misunderstandings of eighth graders of five chemistry concepts found in textbooks. *Journal of Research in Science Teaching*, 29(2), 105-120.
- Abraham, M. R., Williamson, V. M., & Westbrook, S. L. (1994). A cross-age study of the understanding of five chemistry concepts. *Journal of Research in Science Teaching*, 31(2), 147-165.
- Adams, W. K., Reid, S., LeMaster, R., McKagan, S., Perkins, K., Dubson, M., &
  Wieman, C. E. (2008). A study of educational simulations Part II–Interface
  Design. *Journal of Interactive Learning Research*, 19(4), 551-577.
- Akaygun, S. (2009). The effect of computer visualizations on students' mental models of dynamic nature of physical equilibrium. University of Northern Colorado.
- Anderson, D., Lucas, K. B., Ginns, I. S., & Dierking, L. D. (2000). Development of knowledge about electricity and magnetism during a visit to a science museum and related post-visit activities. *Science Education*, 84(5), 658-679.
- Ardac, D., & Akaygun, S. (2004). Effectiveness of multimedia-based instruction that emphasizes molecular representations on students' understanding of chemical change. *Journal of research in science teaching*, 41(4), 317-337.

- Atasoy, B., Akkus, H., & Kadayifci, H. (2009). The effect of a conceptual change approach on understanding of students' chemical equilibrium concepts. *Research in Science & Technological Education*, 27(3), 267-282.
- Baddeley, A. D.; Hitch, G. J. (1974) In *The psychology of learning and motivation*;Bower, G. A., Ed.; Academic Press: New York, 8; pp 47-89.

Baddeley, A. D. (1992). Science, 255, 556-559.

- Baddeley, A. D. (2000) In *The Oxford handbook of memory*; Tulving, E., Craik, F. I. M., Eds.; Oxford University Press: New York ; pp 77-92.
- Baddeley, A. D. (2002). Is working memory still working?. *European psychologist*, 7(2), 85.

Bandura, A. (1977). Social learning theory; Prentice Hall: Englewood Cliffs, NJ.

- Bandura, A. (2001). Social cognitive theory: An agentic perspective. *Annual review of psychology*, *52*(1), 1-26.
- Bandura, A. (1986). *Social foundations of thought and action*; Prentice-Hall: Englewood Cliffs, NJ.
- Ben-Zvi. R., Eylon, B., & Silberstein, J. (1992). Why some students don't learn chemistry: Chemical misconceptions. *Journal of Chemical Education* 69(3), 191.
- Berquist, W., & Heikkinen, H. (1990). Student ideas regarding chemical equilibrium:What written test answers do not reveal. *Journal of chemical Education* 67, 12, 1000.
- Bilgin, İ., & Geban, Ö. (2006). The effect of cooperative learning approach based on conceptual change condition on students' understanding of chemical equilibrium concepts. *Journal of Science Education and Technology*, 15(1), 31-46.

- Bodner, G. M. (1991). I have found you an argument: The conceptual knowledge of beginning chemistry graduate students. *Journal of Chemical Education* 68 (5), 385.
- BouJaoude, S, (2003). Students' systematic errors when solving kinetic and chemical equilibrium problems. Paper presented at the annual meeting of the National Association for Research in Science Teaching, Atlanta, GA., April 15 19, 1993.
  ERIC Document Reproduction Service No. ED 361196.
- Bradley, J. D., & Brand. M. (1985). Stamping out misconceptions. *Journal of Chemical Education* 62 (4), 318.
- Brody, M. (2005). Learning in nature. *Environmental Education Research*, *11*(5), 603-621.
- Brody, M., Bangert, A., & Dillon, J. (2009). Assessing learning in informal science contexts. Commissioned Paper by the National Research Council for Science Learning in Informal Environments Committee.
- Brown, D. E., & Clement, J. (1989). Overcoming misconceptions via analogical reasoning: Abstract transfer versus explanatory model construction. *Instructional science*, 18(4), 237-261.
- Brown, J. S., Collins, A., & Duguid, P. (1989). Situated cognition and the culture of learning. *Educational researcher*, 18(1), 32-42.
- Buckley, B. C. (2000). Interactive multimedia and model-based learning in biology. *International journal of science education*, 22(9), 895-935.

- Bunce, D.M., Gabel, D.L., & Samuel, J. V., (1991). Enhancing Chemistry Problem-Solving Achievement Using Problem Categorization, *Journal of Research in Science Teaching*, 28(6), 505-521.
- Cachapuz, A.F.C. & Maskill, R. (1989). Using word association in formative classroom tests: Following the learning of Le Chatelierís principle. *International Journal of Science Education*, 11, 235-246.
- Canpolat, N., Pınarbaşı, T., Bayrakçeken, S., & Geban, O. (2006). The conceptual change approach to teaching chemical equilibrium. *Research in Science & Technological Education*, 24(2), 217-235.
- Carey, S. (1986). Cognitive science and science education. *American Psychologist*, *41*(10), 1123.
- Chi, M. T. (2008). Three types of conceptual change: Belief revision, mental model transformation, and categorical shift. *International handbook of research on conceptual change*, 61-82.
- Chi, M. T., & Roscoe, R. D. (2002). The processes and challenges of conceptual change. In *Reconsidering conceptual change: Issues in theory and practice* (pp. 3-27).
   Springer Netherlands.
- Chi, M. T., Leeuw, N., Chiu, M. H., & LaVancher, C. (1994). Eliciting self-explanations improves understanding. *Cognitive science*, *18*(3), 439-477.
- Chinn, C. A., & Brewer, W. F. (1993). The role of anomalous data in knowledge acquisition: A theoretical framework and implications for science instruction. *Review of educational research*, 63(1), 1-49.

- Chiu, M. H., Chou, C. C., & Liu, C. J. (2002). Dynamic processes of conceptual change: Analysis of constructing mental models of chemical equilibrium. *Journal of research in science teaching*, 39(8), 688-712.
- Convenience sampling | Lærd Dissertation. (n.d.). Retrieved August 31, 2015, from http://dissertation.laerd.com/convenience-sampling.php
- Creswell, J. W. (2002). *Educational research: Planning, conducting, and evaluating quantitative*. Prentice Hall.
- DeLorenzo R., (1994). Expanded dimensional analysis. *Journal of Chemical Education*. *71*, 789–791.
- Designs for Experiments. (n.d.). Retrieved August 30, 2015, from http://web.csulb.edu/~msaintg/ppa696/696exper.htm
- Deters, K. M. (2003). What should we teach in high school chemistry?." *Journal of chemical education*, 80(10), 1153.
- Dimitrov, D. M., & Rumrill, P. D. (2003). Pretest-posttest designs and measurement of change. Work-and over Medical Publishers Incorporated then IOS Press-, 20(2), 159-165.
- DiSessa, A. A. (1993). Toward an epistemology of physics. *Cognition and instruction*, *10*(2-3), 105-225.
- Disessa, A. A. (2002). Why "conceptual ecology" is a good idea. In *Reconsidering conceptual change: Issues in theory and practice* (pp. 28-60). Springer Netherlands.
- Disessa, A. A., & Sherin, B. L. (1998). What changes in conceptual change?. *International journal of science education*, 20(10), 1155-1191.

- Doymus, K. (2008). Teaching chemical equilibrium with the jigsaw technique. *Research in Science Education*, *38*(2), 249-260.
- Dugard, P., & Todman, J. (1995). Analysis of pre-test-post-test control group designs in educational research. *Educational Psychology*, *15*(2), 181-198.
- Duit, R. (2009). Bibliography—STCSE Students' & teachers' conceptions and science education. Retrieved July 2009 from <u>http://www.ipn.uni-</u> kiel.de/aktuell/stcse/stcse.html
- Duit, R., & Treagust, D. F. (2003). Conceptual change: a powerful framework for improving science teaching and learning. *International journal of science education*, 25(6), 671-688.
- Duschl, R. A., & Gitomer, D. H. (1991). Strategies and challenges to changing the focus of assessment and instruction in science classrooms. *Educational Assessment*, 4(1), 37-73.
- Duschl, R., Schweingruber, H., & Shouse, A. (Eds.). (2007). Taking science to school: Learning and teaching science in grades k-8. Washington, DC: National Academy Press.
- Engel, R. J., & Schutt, R. K. (2014). *Fundamentals of social work research*. Sage Publications.
- Erdfelder, E., Faul, F., & Buchner, A. (1996). GPOWER: A general power analysis program. *Behavior research methods, instruments, & computers, 28*(1), 1-11.
- Erduran, S., Simon, S., & Osborne, J. (2004). TAPping into argumentation:Developments in the application of Toulmin's argument pattern for studying science discourse. *Science education*, 88(6), 915-933.

Falk, J. H., & Dierking, L. D. (1992). The museum experience. Howells House.

- Falk, J., Brooks, P., & Amin, R. (2001). Investigating the long-term impact of a science center on its community: The California Science Center LASER Project. *Freechoice science education: How we learn science outside of school*, 115-132.
- Gabel, D. L., (1993). Use of the Particle Nature of Matter in Developing Conceptual Understanding. *Journal of Chemical Education*, 70(3), 193-194.
- Gilbert, J. K. (2005). *Visualization in Science Education*. Springer: Dordrecht, The Netherlands.
- Gizmos. (2015, January 15). Retrieved from http://www.explorelearning.com/
- Gorsky, P., & Finegold, M. (1992). Using Computer Simulation to Restructure Students' Conceptions of Force. *Journal of Computers in Mathematics and science teaching*, 11(2), 163-78.
- Gregorius, R. M. Simulation Excerpts.

http://www3.canisius.edu/~gregorir/ic2home/ebookexcerpts/ (January 2015).

- Gupta, A., & Fisher, D. (2012). Technology-supported learning environments in science classrooms in India. *Learning Environments Research*, *15*(2), 195-216.
- Greenbowe, J. T. & Windschitl, A. M. (1998). Developing and using conceptual computer animations for chemistry instruction. *Journal of Chemical Education* 75(12),1658.
- Gabel, L. D., Samuel, V. K., & Hunn. D. (1987). Understanding the particulate nature of matter. *Journal of chemical Education*, 64(8), 695.
- Gall, M. D., Borg, W. R., & Gall, J. P. (1996). *Educational research: An introduction*.Longman Publishing.

- Gay, L. R., & Airasian, P. (2003). Educational research: Competencies for analysis and application (7th ed.). Upper Saddle River, NJ: Pearson Education.
- Glassman, S. (1967). High school students' ideas with respect to certain concepts related to chemical formulas and equations. *Science Education*, *51*(1), 84-103.
- Glynn, S.M. (1991). Explaining science concepts: A teaching-with-analogies model. In S.Glynn, R. Yeany and B. Britton (Eds.), The psychology of learning science (pp. 219-240). Hillsdale, NJ, Erlbaum.
- Griffiths, A. K., & Preston, K. R. (1992). Grade-12 students' misconceptions relating to fundamental characteristics of atoms and molecules. *Journal of Research in Science Teaching*, 29(6), 611-628.
- Hameed, H., Hackling, M. W., & Garnett, P. J. (1993). Facilitating conceptual change in chemical equilibrium using a CAI strategy. *International Journal of Science Education*, 15(2), 221-230.
- Harrison, A. G., & Treagust, D. F. (2002). The particulate nature of matter: Challenges in understanding the submicroscopic world. In J. K. Gilbert, O. D. Jong, D. F.
- Hein, G. E. (2002). Learning in the Museum. Routledge.
- Herron, D. J. (1975). Piaget for chemists. Explaining what" good" students cannot understand." *Journal of Chemical Education* 52(3), 146.
- Hoban, R. A., Finlayson, O. E., & Nolan, B. C. (2013). Transfer in chemistry: a study of students' abilities in transferring mathematical knowledge to chemistry. *International Journal of Mathematical Education in Science and Technology*, 44(1), 14-35.

Hogan, K. N. (2010). BK and PRESSLEY, M. 2000. Discourse Patterns and Collaborative Scientific Reasoning in Peer and Teacher–Guided Discussions. www. incommunity research. org/about/.../bnastasiful. htm. Retrieved: July.

- Huck, S. W., & McLean, R. A. (1975). Using a repeated measures ANOVA to analyze the data from a pretest-posttest design: A potentially confusing task.*Psychological Bulletin*, 82(4), 511.
- Hull, G. A., & Greeno, J. G. (2006). Identity and agency in nonschool and school worlds. *Counterpoints*, 77-97.
- Johnson, R. B., & Onwuegbuzie, A. J. (2004). Mixed methods research: A research paradigm whose time has come. *Educational researcher*, *33*(7), 14-26.
- Johnson, B., & Christensen, L. (2008). Educational research: Quantitative, qualitative, and mixed approaches. Sage.
- Johnson, P., & Tymms, P. (2011). The emergence of a learning progression in middle school chemistry. *Journal of Research in Science Teaching*, *48*(8), 849-877.
- Johnstone, A. H. (1974). Evaluation of chemistry syllabuses in Scotland. *Studies in Science Education*, 1(1), 21-49.
- Johnstone, A. H. (1984). New stars for the teacher to steer by?. *Journal of Chemical Education* 61 (10), 847.
- Johnstone, A. H. (1993). The development of chemistry teaching: A changing response to changing demand. *Journal of Chemical Education*, 70(9), 701-704.
- Johnstone, A.H., MacDonald, J.J., & Webb, G., (1977). Chemical Equilibrium and its Conceptual Difficulties, *Education in Chemistry*, *14*(6), 169-171

- Jonassen, D. H., & Hung, W. (2006). Learning to troubleshoot: A new theory-based design architecture. *Educational Psychology Review*, *18*(1), 77-114.
- Kalainoff, M., Lachance, R., Riegner, D., & Biaglow, A. (2012). A computer algebra approach to solving chemical equilibria in general chemistry. *PRIMUS*, 22(4), 284-302.
- Kautz, C. H., Heron, P. R., Shaffer, P. S., & McDermott, L. C. (2005). Student understanding of the ideal gas law, Part II: A microscopic perspective. *American Journal of Physics*, 73(11), 1064-1071.
- Kemper, E. A., Stringfield, S., & Teddlie, C. (2003). Mixed methods sampling strategies in social science research. *Handbook of mixed methods in social and behavioral research*, 273-296.
- Khan, S. (2007). Model-based inquiries in chemistry. Science Education, 91(6), 877-905.
- Kousthana, M. & Tsaparlis, G. (2002). Students errors in solving numerical chemical equilibrium problems. *Chemistry Education:Research and Practice in Europe*, 3(3), 517.
- Kozma, R. & Russell, J. (1997). Multimedia and understanding: Expert and Novice responses to different representations of chemical phenomena. *Journal of Research in Science Teaching*, 43(9), 949-968.
- Krajcik, J. S. (1989). Paper presented at the American Anthropological Association, Washington, DC.
- Krishnamurthi, A., Alliance, A., & Rennie, L. J. Informal Science Learning and Education: Definition and Goals.

- Leinhardt, G., Tittle, C., and Knutson, K. (2000). *Talking to Oneself: Diaries of Museum Visits*. Retrieved August 30, 2015 from http://mlc.lrdc.pitt.edu/mlc.
- Leopold D. G. and Edgar B., (2008), Degree of Mathematics Fluency and Success in Second-Semester Introductory Chemistry, *Journal of Chemical Education*, 85, 724–73.
- Lewalter, D. (2003). Cognitive strategies for learning from static and dynamic visuals. *Learning and Instruction*, *13*(2), 177-189.
- Lin, H., Cheng, H., & Lawrenz, F. (2000) The assessment of students and teachers' understanding of gas laws. *Journal of Chemical Education*. 77(2), 235–238.
- Linn, R. L., & Slinde, J. A. (1977). The determination of the significance of change between pre-and posttesting periods. *Review of Educational Research*, 121-150.
- Liu, X., & Lesniak, K. M. (2005). Students' progression of understanding the matter concept from elementary to high school. *Science Education*, 89(3), 433-450.
- Lowe, R. K. (2003). Animation and learning: selective processing of information in dynamic graphics. *Learning and instruction*, *13*(2), 157-176.
- Lewis, J. (1933), Analogies in teaching freshman chemistry, *Journal of Chemical Education*, 10, 627-630
- Mathewson, J. H. (1999). Visual-spatial thinking: An aspect of science overlooked by educators. *Science Education*, *83*(1), 33-54.
- Mayer, R. E. (2001). *Multimedia learning*; Cambridge University Press: Oxford.
- Mayer, R. E., Bove, W., Bryman, A., Mars, R, & Tapangco, L. (1996). Why less is more: Meaningful learning from visual and verbal summaries of science textbook lessons. Journal of Educational Psychology, 88 (1), 64-73.

- Mayer, R. E., & Moreno, R. (2002). Animation as an aid to multimedia learning. *Educational psychology review*, *14*(1), 87-99.
- McMillan, J. H., & Schumacher, S. (1984). *Research in education: A conceptual introduction*. Little, Brown.

Mertler, C. A., & Charles, C. M. (2005). *Introduction to educational research*. Pearson/A & B.

Miller, G. A. (1956). Psychological Review, 63, 81-97.

- Moorehead, C. (n.d.). Retrieved August 31, 2015, from
  - http://www.dartmouth.edu/~oir/docs/Types\_of\_Experimental\_Designs\_Handout.
- Myers, J.L. & Well, A.D. (1991) *Research Design and Statistical Analysis* (New York, HarperCollins).
- Nakhleh, M., & Mitchell, R. (1993). Concept learning versus problem solving. *Journal of Chemical Education*, 70, 190 - 192.
- Niaz, M. (1995). Cognitive conflict as a teaching strategy in solving chemistry problems:
   A dialectic–constructivist perspective. *Journal of research in science teaching*, 32(9), 959-970
- Niedzielski, R., & Walmsley, F. (1982). What do incoming freshman remember from high school chemistry. *Journal of Chemical Education*, *59*, 149-151.
- Nakleh, M. B. (1992). Why some students don't learn chemistry: Chemical misconceptions. *Journal of Chemical Education* 69(3), 191.
- Onwuegbuzie, A. J., & Leech, N. L. (2007). A call for qualitative power analyses. *Quality & Quantity*, *41*(1), 105-121.

- Onwuegbuzie, A. J., & Collins, K. M. (2007). A typology of mixed methods sampling designs in social science research. *The qualitative report*, *12*(2), 281-316.
- Özdemir, G., & Clark, D. B. (2007). An overview of conceptual change theories. *Eurasia Journal of Mathematics, Science & Technology Education*, *3*(4), 351-361.
- Özmen, H. (2007). The effectiveness of conceptual change texts in remediating high school students' alternative conceptions concerning chemical equilibrium. *Asia Pacific Education Review*, 8(3), 413-425.
- Paivio, A. (1986). *Mental representations: A dual-coding approach*; Oxford University Press: Oxford.
- Posner, G. J., Strike, K. A., Hewson, P. W., & Gertzog, W. A. (1982). Accommodation of a scientific conception: Toward a theory of conceptual change. *Science education*, 66(2), 211-227.
- Quilez, J. (2004). A historical approach to the development of chemical equilibrium through the evolution of the affinity concept: some educational suggestions. *Chem. Educ. Res. Pract.*, 5(1), 69-87.
- Raviolo, A., & Garritz, A. (2009). Analogies in the teaching of chemical equilibrium: a synthesis/analysis of the literature. *Chemistry Education Research and Practice*, 10(1), 5-13.
- Raviolo, A. (2012). Using a Spreadsheet Scroll Bar to Solve Equilibrium Concentrations. *Journal of Chemical Education*, 89(11), 1411-1415.
- Rieber, L. P. (1990). Animation in computer-based instruction. *Educational Technology Research and Development*, 38 (1), 77-86.

- Rieber, L. P. (1991). Animation, incidental learning, and continuing motivation. *Journal of Educational Psychology*, *83*(3), 318.
- Resnick, M.: Turtles, termites, and traffica jams: explorations in massively parallel microworlds; MIT Press: Cambridge, 1994.
- Russell, W. J. & Kozma, B. R. (1994). 4M: Chem-multimedia and mental models in chemistry. *Journal of Chemical Education* 71(8), 669.
- Russell, M. J. (1988). Simple models for teaching equilibrium and Le Chatelier's principle. *Journal of Chemical Education*, 65(10), 871.
- Russell, J., Kozma, R., Jones, T., Wykoff, J., Marx, N., & Davis, J. (1997). Use of simultaneous synchronized macroscopic, microscopic, and symbolic representations to enhance the teaching and learning of chemical concepts. Journal of Chemical Education, 74, 330–334.
- Russell, J., & Kozma, R. (2005). Assessing Learning from the Use of Multimedia
  Chemical Visualization Software. In *Visualization in science education* (pp. 299-332). Springer Netherlands.
- Schnotz, W. (1998), Conceptual Change, in D. H. Rost, ed., `Handwörterbuch Pädagogische Psychologie', Psychologie Verlags Union, Weinheim, pp. 75-81.
- Schnotz, W., Vosniadou, S. & Carretero, M., eds (1999), New Perspectives on Conceptual Change, Pergamon, Oxford
- Siebert, H. (2003), Pädagogischer Konstruktivismus Lernen als Konstruktion von Wirklichkeit, Luchterhand, München/Unterschleiÿheim.
- Siebert, H. (2003), Pädagogischer Konstruktivismus Lernen als Konstruktion von Wirklichkeit, Luchterhand, München/Unterschleiÿheim.

- Sanger, M. J., Brecheisen, D. M., & Hynek, B. M. (2001). Can computer animations affect college biology students' conceptions about diffusion & osmosis?. *The American Biology Teacher*, 63(2), 104-109.
- Sawrey, B.A., (1990). Concept-Learning Versus Problem Solving Revisited, *Journal of Chemical Education*, 67(3), 253-254.
- Scott, F. J. (2012). Is mathematics to blame? An investigation into high school students' difficulty in performing calculations in chemistry. *Chemistry Education Research and Practice*, *13*(3), 330-336.
- Shayer, M. (1991). Improving standards and the national curriculum . *School Science Review*, 72 (260), 15-24.
- Skemp, R. R. (1976). Relational understanding and instrumental understanding. *Mathematics teaching*, 77, 20-26.
- Smith III, J. P., Disessa, A. A., & Roschelle, J. (1994). Misconceptions reconceived: A constructivist analysis of knowledge in transition. *The journal of the learning sciences*, 3(2), 115-163.
- Sweller, J. (1994). Cognitive load theory, learning difficulty, and instructional design. *Learning and instruction*, *4*(4), 295-312.
- Spencer, E. H. (1996). Mathematical SAT test scores and college chemistry grades." *Journal of Chemical Education*, 73(12), 1150.
- Stark, R. (2002), Conceptual Change: kognitivistisch oder kontextualistisch? Technical Rep ort 149, Ludwig-Maximilians-Universität, Lehrstuhl für Empirische Pädagogik und Pädagogische Psychologie.

Strike, K. A., & Posner, G. J. (1992). A revisionist theory of conceptual change. Philosophy of science, cognitive psychology, and educational theory and practice, 147-176.

- Stevens, S. Y., Shin, N., & Krajcik, J. S. (2009). Towards a model for the development of an empirically tested learning progression. In *Learning Progressions in Science* (*LeaPS*) Conference, Iowa City, IA.
- Taber, K. S., (2002). Alternative Conceptions In Chemistry: Prevention, Diagnosis And Cure? London: The Royal Society of Chemistry.

Taber, K. S. (2009). Learning at the symbolic level. In *Multiple representations in chemical education* (pp. 75-105). Springer Netherlands.

- Tao, P. K., & Gunstone, R. F. (1999). The process of conceptual change in force and motion during computer-supported physics instruction. *Journal of Research in Science Teaching*, 36(7), 859.
- Treagust, D. F., & Chittleborough, G. (2001). Chemistry: A matter of understanding representations. *Advances in research on teaching*, *8*, 239-268.
- Treagust, F. D., Tyson, L., & Bucat, B. R. (1999). The complexity of teaching and learning chemical equilibrium. *Journal of Chemical Education* 76(4), 554-558.
- Treagust,&J. H. van Driel (Eds.), Chemical education: Toward research-based practice (pp. 189–212).
- Trey, L., & Khan, S. (2008). How science students can learn about unobservable phenomena using computer-based analogies. *Computers & Education*, 51(2), 519-529.

- Tversky, B., Morrison, J. B., & Betrancourt, M (2002). Animation: Can it facilitate? International Journal of Human Computer Studies. International *Journal of Human Computer Studies*, 57, 247-262.
- Trundle, K. C., & Bell, R. L. (2005). The use of a computer simulation to promote scientific conceptions of moon phases. In Annual Meeting of the National Association of Research in Science Teaching, Dallas, TX.

University of Colorado at Boulder PhET: Interactive Simulations. http://phet.colorado.edu/index.php (January 15, 2015),

- Van Driel, J. H., & Gr\u00e4ber, W. (2003). The teaching and learning of chemical equilibrium. In *Chemical education: Towards research-based practice* (pp. 271-292). Springer Netherlands.
- Vosniadou, S., & Brewer, W. F. (1992). Mental models of the earth: A study of conceptual change in childhood. *Cognitive psychology*, 24(4), 535-585.
- Vosniadou, S. (1994). Capturing and modeling the process of conceptual change. *Learning and instruction*, *4*(1), 45-69.
- Vosniadou, S., & Ioannides, C. (1998). From conceptual development to science education: A psychological point of view. *International Journal of Science Education*, 20(10), 1213-1230.
- Vosniadou, S. (2001). What can persuasion research tell us about conceptual change that we did not already know?. *International Journal of Educational Research*, 35(7), 731-737.

- Vosniadou, S., Ioannides, C., Dimitrakopoulou, A., & Papademetriou, E. (2001).
   Designing learning environments to promote conceptual change in science.
   *Learning and instruction*, 11(4), 381-419.
- Vosniadou, S. (2002). Mental models in conceptual development. In *Model-Based Reasoning* (pp. 353-368). Springer US.

Vosniadou, S. (2007). Conceptual change and education. Human Development, 50(1), 47.

- Weisman, L. R. (1981). A mathematics readiness test for prospective chemistry students. *Journal of Chemical Education* 58 (7), 564. 27(10), 1053-1065.
- Widodo, A., & Duit, R. (2004). Konstruktivistische Sichtweisen vom Lehren und Lernen und die Praxis des Physikunterrichts. Zeitschrift f
  ür Didaktik der Naturwissenschaften, 10, 233-255.
- Williamson, V. M., & Abraham, M. R. (1995). The effects of computer animation on the particulate mental models of college chemistry students. *Journal of Research in Science Teaching*, 32(5), 521-534.
- Yezierski, J. E., & Birk, P. J. (2006) "Misconceptions about the particulate nature of matter. Using animations to close the gender gap." *Journal of Chemical Education* 83(6), 954.
- Zimmerman, D. W., & Williams, R. H. (1982). Gain scores in research can be highly reliable. *Journal of Educational Measurement*, *19*(2), 149-154.
- Zoller, U. (1990). Students' misunderstandings and misconceptions in college freshman chemistry (general and organic). *Journal of Research in Science Teaching*, 27(10), 1053-1065.

## **Bharath Sampath Kumar**

## **Education**

<b>Doctor of Philosophy in Educational Sciences -STEM Education</b> University of Kentucky, Lexington, KY	Expected			
<b>Dissertation Title:</b> Evaluating Role of Interactive Visualization Tool in Improving Students' Conceptual Understanding of Chemical Equilibrium. <b>Advisor:</b> Dr. Rebecca Krall				
Master of Arts Secondary Science Education West Virginia University, Morgantown, WV	2012			
Advisor: Dr. Patricia Obenauf				
<b>Certificate in University Teaching</b> West Virginia University, Morgantown, WV	2012			
Advisor: Dr. Constinia Charbonette				
<b>Master of Science – Analytical Chemistry</b> Washington State University, Pullman, WA	2007			
<i>Thesis title:</i> Electrospray ion mobility spectrometry for the separation and detection of explosives and anions in aqueous samples <i>Advisor:</i> Dr. Herbert H. Hill				
Master of Science – Inorganic Chemistry Loyola College, Chennai, India	2002			
<b>Thesis title:</b> Electrical and humidity sensing properties of Molybdenum (VI Tungsten (VI) oxide composites <b>Advisor:</b> Dr. K.S. Nagaraja	I) oxide and			
Bachelor of Science - Chemistry Loyola College, Chennai, India	2000			

Advanced Diploma in Computer Applications Loyola Institute of Business Administration, Chennai, India	<b>1998</b>				
<b>Diploma in Computer Applications</b> Loyola Institute of Business Administration, Chennai, India	a <b>1997</b>				
<b>Continuing Education</b>					
Johns Hopkins University (via Coursera.com)					
R – Programing Certificate	August 2016				
<b>Higher Education Work Experience</b>					
Kentucky State University, Frankfort, KY	Fall 2016-current				
Adjunct Professor - Chemistry					
University of Kentucky, Lexington, KY	Fall 2015- Spring 2016				
Graduate Research Assistant- UKY Evaluation Center					
Graduate Assistant – OTIS Management & NCATE data analysis					
University of Kentucky, Lexington, KY	Spring & Summer 2014				
Graduate Assistant – Physics Curriculum Development					
University of Kentucky, Lexington, KY	Summer 2014				
Graduate Teaching Assistant – Physics Laboratories (P	HY 211)				
University of Kentucky, Lexington, KY	Fall 2012- Fall 2013				
Graduate Research Assistant - Chemistry					
West Virginia University, Morgantown, WV	August 2011 – May 2012				
Graduate Teaching Assistant - Chemistry					
West Virginia University, Morgantown, WV	August 2010 – May 2011				
Graduate Research Assistant - Chemistry					
Washington State University, Pullman, WA	August 2006 – May 2007				
Graduate Teaching Assistant - Chemistry					
Washington State University, Pullman, WA	August 2005 – August 2006				

## K-12 Work Experience

GEAR UP Summer Academy – InstructorUniversity of Kentucky, Lexington, KYSummer 2015 & 2016Robinson Scholar Program - High school statistics, physics and chemistry instructorUniversity of Kentucky, Lexington, KYSummer 2013, 2014, 2015 & 2016STEAM Academy – Chemistry InstructorUniversity of Kentucky, Lexington, KYSpring 2014AP & SAT Chemistry InstructorPrime Academy Inc. Irvine, CAOctober 2007 to July 2008

## Awards

1<sup>st</sup> place, Graduate Research Presentation Award, Kentucky Academy of Science,

Morehead KYNovember 2013West Virginia University Provost FellowshipAugust 2011- May 2012

## **Publications**

- Kanu, A. B., Kumar, B. S., & Hill, H. H. (2012). Evaluation of micro-versus nanoelectrospray ionization for ambient pressure ion mobility spectrometry. *International Journal for Ion Mobility Spectrometry*, 15(1), 9-20.
- Abraham, A., Mihaliuk, E., Kumar, B., Legleiter, J., & Gullion, T. (2010). Solid-state NMR study of cysteine on gold nanoparticles. *The Journal of Physical Chemistry C*, *114*(42), 18109-18114.
- Kumar, B., Pifer, P. M., Giovengo, A., & Legleiter, J. (2010). The effect of set point ratio and surface Young's modulus on maximum tapping forces in fluid tapping mode atomic force microscopy. *Journal of Applied Physics*, 107(4), 044508.

## Work in progress

Kumar, B., Legleiter. J. Mechanical and Surface Properties of *Borrelia burgdorferi* using Tapping Mode Atomic Force microscopy and Scanning Probe Acceleration Microscopy. (Manuscript in progress).

## **Presentations**

#### <u>National</u>

- Sampath Kumar, B. & Krall, R. (2016, August). *Effect of dynamic simulations on students' understanding of chemical equilibrium.* Paper accepted at the Bicentennial Chemical Education Conference, Greeley, CO.
- Sampath Kumar, B. & Krall, R. (2016, August). Evaluating the role of visualization tool such as simulation towards students' conceptual understanding of chemical equilibrium. Paper accepted at, 252nd ACS National Meeting, Philadelphia, PA.
- LeVaughn, J., Krall, R. M., Kumar, B. S., Wilhelm, J., & Hanley, C. (2016, April). From professional development to teacher practice: project-based investigations of local watersheds. Poster presented at the annual meeting for the National Association for Research in Science Teaching, Baltimore, MD.
- Krall, R. M., LeVaughn, J. Kumar, B. S. (2016, April). A Comparison of Three Teacher-Created Project-Based Investigations on Local Watersheds: Successes and Limitations. Paper presented at the annual meeting for the National Association for Research in Science Teaching, Baltimore, MD.
- Sampath Kumar, B. & Krall, R. (2014, November). *Improving Learning of Chemical Equilibrium with Technology*. Presentation, School Science and Mathematics Conference, Jacksonville, FL.
- Sampath Kumar, B. & Krall, R. (2014, August). *Teaching chemical equilibrium with technology*. Paper accepted at the Bicentennial Chemical Education Conference, Grand Rapids, MI.
- Herbert H. Hill, Maggie Tam, Bharath Kumar, Prabha Dwivedi, Abu B. Kanu (2007, February). Detection of Explosives in Liquids by Electrospray Ion Mobility Spectrometry, 58<sup>th</sup> Pittsburgh Conference on Analytical Chemistry & Applied Spectroscopy, *Chicago, Illinois, USA*

#### **Regional**

Sampath Kumar, B. & Krall, R. (2015, October). *Teaching Chemical Equilibrium with Technology*. Presentation, Mid-Atlantic ASTE Regional Conference, Lore City OH.

#### <u>State</u>

- Kumar, B. S., & Krall, R. M. (2014, November). *Teaching chemical equilibrium with technology*. Paper presented at the annual meeting of the Kentucky Academy of Science. Lexington, KY.
- Kumar, B., & Krall, R. M. (2013, November). Using Technology to Teach Chemical Equilibrium. Paper presented at the annual meeting of the Kentucky Academy of Science. Morehead, KY.

#### Non-refereed presentations

- Kumar, B. S., & Legleiter, J. (2010, April). Mechanical and Surface Properties of Borrelia burgdorferi using Tapping Mode Atomic Force microscopy and Scanning Probe Acceleration Microscopy. Poster presentation at the WVNano Initiative Research Symposium, Morgantown, WV.
- Kumar, B. S., & Legleiter, J. (2010, March). Mechanical and Surface Properties of Borrelia burgdorferi using Tapping Mode Atomic Force microscopy and Scanning Probe Acceleration Microscopy. Poster presentation at the Research Horizon Poster Symposium, Morgantown, WV.
- Kumar, B. S., & Legleiter, J. (2010, March). Effect of set point ratio and surface Young's modulus on maximum tapping forces in atomic force microscope (AFM). Poster presentation at the American Chemical Society Student Affiliates, Morgantown, WV.