



Chemistry
Education Research
and Practice

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Journal:	<i>Chemistry Education Research and Practice</i>
Manuscript ID	RP-ART-03-2022-000063.R1
Article Type:	Paper
Date Submitted by the Author:	14-Apr-2022
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Title

ChemSims: Using simulations and screencasts to help students develop particle-level understanding of equilibrium in an online environment before and during COVID

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Abstract

Equilibrium is a challenging concept for many, largely because developing a deep conceptual understanding of equilibrium requires someone to be able to connect the motions and interactions of particles that cannot be physically observed with macroscopic observations. Particle level chemistry animations and simulations can support student connections of particle motion with macroscopic observations, but for topics such as equilibrium additional visuals such as graphs are typically present which add additional complexity. Helping students make sense of such visuals requires careful scaffolding to draw their attention to important features and help them make connections between representations (e.g., particle motion and graphical representations). Further, as students enter our classrooms with varying levels of background understanding, they may require more or less time working with such simulations or animations to develop the desired level of conceptual understanding. This paper describes the development and testing of activities that use the PhET simulation “Reactions and Rates” to introduce the concept of equilibrium as a student preclass activity either in the form of directly using the simulation or guided by an instructor through a screencast. The pre-post analysis of the two most

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2
3 recent implementations of these activities indicate that students show improved understanding of
4 the core ideas underlying equilibrium regardless of instructor, institution, or type of instructional
5 environment (face to face or remote). We also observed that students were more readily able to
6 provide particle level explanations changes in equilibrium systems as they respond to stresses
7 (such as changes to concentration and temperature) if they have had prior course instruction on
8 collision theory. Lastly, we observed that student answers to explain how an equilibrium will
9 respond to an applied stress more often focus on either initial responses or longer-term stability
10 of concentrations, not on both key aspects.
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23 **Introduction**

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25 Students enter our introductory college science classes with a variety of background experiences
26 and abilities. For some students, introductory science courses are largely a review from high
27 school while for others it is the first time they are encountering the material. Further, some
28 students may require more or less time to process material. This is one of the rationale for
29 “flipped” classrooms where students engage in some kind of activity on their own prior to class
30 (readings, watching videos, etc.) and then spend class time working through homework problems
31 (Abeysekera and Dawson, 2015). The popularity of the flipped classroom has grown
32 substantially in the last decade as evidenced by fewer than 20 articles focused on flipped
33 classroom published in science education journals in 2010, to over 100 in 2018, and over 200 for
34 the years 2020 and 2021. Of those published in 2020-2021, 31 focused specifically on chemistry
35 education (Eichler, 2022). Unfortunately, the traditional version of the flipped classroom, where
36 students watch lecture videos outside of class and do homework type problems in class, suffers
37 from the same issues as the traditional lecture (Bancroft, Jalaeian and John, 2021). In a recent
38 commentary on the future of the flipped classroom, Eichler encourages the chemistry education
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3 community to, “transition the focus from probing the general efficacy of the flipped classroom to
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5 investigating how the preclass learning and in-person instruction can be optimized to address
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7 chemistry-specific learning objectives.” Determining the key features of effective preclass
8
9 learning activities is critical given that although the stated impetus for implementing a flipped
10
11 classroom is often the incorporation of more active learning during the in-class instruction,
12
13 research studies have shown that improved student outcomes depend largely on the preclass
14
15 activities (Eichler and Peeples, 2016; Rau *et al.*, 2017; Bancroft, Jalaean and John, 2021).
16
17 Passive lectures, whether in class or outside of class via video, have been repeatedly shown to
18
19 have very little impact on student learning (Koedinger *et al.*, 2015). However, incentivizing
20
21 students’ active engagement in activities that support their development of conceptual
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23 understanding have been found to increase student achievement (Chi and Wylie, 2014; Bancroft,
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25 Jalaean and John, 2021). The use of such activities in college classes have been sometimes been
26
27 shown to result in lower student perceptions of learning and enjoyment (Deslauriers *et al.*, 2019),
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29 but in the recent emergency shift to remote teaching caused by the COVID-19 pandemic, it was
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31 these types of activities that resulted in increased student perceptions of enjoyment and learning
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33 (Nguyen *et al.*, 2021).
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42 This paper focuses on the development and evaluation of activities designed to actively engage
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44 students in the construction of a conceptual understanding of equilibrium systems and to be
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46 completed by students outside of the classroom prior to any formal in-class instruction. These
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48 activities are designed to provide students with an introduction to dynamic equilibrium systems
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50 by scaffolding their interactions with a particle-level simulation. Equilibrium is typically a
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52 challenging concept in chemistry (Bergquist and Heikkinen, 1990; Cheung, 2009) and providing
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3 students an opportunity to engage with this concept outside of the classroom allows them to
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5 work through the material at their own pace as well as provides a common experience that
6
7 instructors can build on during in class instruction. However, appropriate scaffolding is critical
8
9 as students interacting with complex simulations on their own can result in them missing or
10
11 misinterpreting key elements of the simulation (Hegarty, 2004). Thus, an alternative to students'
12
13 independent interactions with the simulation is students viewing a screencast in which an
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15 instructor manipulates the simulation and provides some narration to highlight key elements of
16
17 the simulation for students (Herrington, Sweeder and VandenPlas, 2017; Martinez *et al.*, 2021).
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19 As there are potential benefits and challenges to both independent simulation manipulation and
20
21 watching of a screencast (Mayer and Moreno, 2003; Hegarty, 2004; Keehner *et al.*, 2008), we
22
23 aim to identify the key challenges that students have in using these activities outside of class to
24
25 develop a particle-level understanding of equilibrium, as well as any differences that exist
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27 between students who use the simulation compared with those who watch the screencast.
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29 Further, as we were in the middle of this study when the COVID-19 hit, we were able to
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31 compare student learning gains using these materials to support a face-to-face class as compared
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33 to their use in a class that had transitioned to emergency remote instruction, and to determine
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35 how the necessary modifications of some questions when switching to a fully online delivery
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37 impacted information obtained from student responses.
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46 **Background**

47 *Student understanding of equilibrium*

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49 Equilibrium is a challenging concept for students because of its abstract nature; though students
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51 may be able to solve algorithmic equilibrium problems, they often struggle to be able to provide
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53 correct reasoning about equilibrium systems (Quílez-Pardo and Solaz-Portolés, 1995;
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3 Karpudewan *et al.*, 2015). In teaching equilibrium, there are several common, non-productive
4 ideas that students have been found to consistently hold. These include ideas that: reactions stop
5 at equilibrium or that concentrations of products and reactants are equal at equilibrium
6
7 (Demircioğlu, Demircioğlu and Yadigaroglu, 2013); the forward and reverse reactions are
8 oscillatory rather than occurring simultaneously (Driel, Verloop and Vos, 1998); there is a
9 difference between reaction rate and extent of reaction (Erdemir, Geban and Uzuntiryaki, 2000);
10 and reactions must go to completion before the reversing (Al-Balushi *et al.*, 2012). One key
11 factor that may contribute to the difficulty students have in understanding the concept of
12 equilibrium is their inability to physically see what is happening to the particles so they can
13 connect particle motion to the macroscopic observations (Lekhavat and Jones, 2009; Ganasen
14 and Shamuganathan, 2017).

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31 One way to help students visualize abstract chemical concepts at the particulate level is through
32 the use of animations and simulations (Nakhleh, 1992; Sanger, Phelps and Fienhold, 2000; Kelly
33 and Jones, 2007). Viewing particle motion and interactions involved in chemical phenomena
34 have been successful in helping students develop a better understanding of chemical equilibrium
35 (Akaygun and Jones, 2014; Ganasen and Shamuganathan, 2017), and are most useful when they
36 are short, visually appealing, and cover material at the desired specificity and context (Burke,
37 Greenbowe and Windschitl, 1998; Suits and Sanger, 2013). As chemical equilibrium is one of
38 the more difficult concepts to master and has applications in several other chemistry concepts
39 (Bergquist and Heikkinen, 1990), it is critical that students develop scientifically accurate mental
40 models, and simulations may be a powerful pedagogical tool in supporting this development.
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3 Something else that may contribute to students' and instructors' difficulty with equilibrium is the
4 overreliance on Le Chatelier's principle (LCP) to explain changes in equilibrium systems
5
6 (Cheung, 2009). Using LCP to predict or justify shifts in an equilibrium system resulting from
7
8 external stresses (such as changes to concentration and temperature), without an underlying
9
10 understanding of how such stresses affect the concentrations and interactions of the particles, is
11
12 akin to applying an algorithm to solve a problem without understanding why. Many curricula
13
14 rely heavily on Le Chatelier's principle to explain how an equilibrium system responds to
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16 stresses, as opposed to collision theory or the reaction quotient, the basis for particle interactions
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18 and concentration (Cheung, 2009).
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26 *Use of Simulations and Screencast in Online Learning*

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28 The constructivist theory of learning posits that learning occurs as individuals use experience to
29
30 build new knowledge structures or integrate experiences into existing knowledge structures
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32 (Bodner, 1986). As Seery (2015) notes in his evaluation of flipped learning in college chemistry
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34 courses, "teaching under the umbrella of constructivism would therefore mean that teachers don't
35
36 just tell students what they need to know, but provide structured activities so that students can
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38 develop their knowledge within the parameters of their own prior understanding." In chemistry,
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40 coherent conceptual knowledge requires understanding phenomena at three different levels, the
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42 macroscopic (what we can observe with our eyes), the symbolic (chemical equations), and the
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44 particle (atoms, molecules, ions) levels (Johnstone, 1991; Liu and Lesniak, 2005; Adbo and
45
46 Taber, 2009; Taber, 2013). This is often particularly challenging for students as atoms, ions, and
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48 molecules are far too small to be seen with our eyes, even with very powerful microscopes.
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50 Thus, a particle-level understanding of phenomena requires students to be able to imagine in
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52 their heads how particles are moving and interacting to develop a mental model. Using
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3 animations or simulations in the classroom have been shown to help students develop such
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5 mental models of chemical processes at the particle level (Williamson and Abraham, 1995).
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7 Typically, when used in class, an instructor will help students to focus on and understand the
8
9 aspects of the simulation that can assist in the creation of productive mental models (Mayer and
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11 Anderson, 1991). In the ChemSims project (ChemSims, no date), we have built on these ideas by
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13 developing outside-of-class activities where students engage with such simulations using
14
15 carefully scaffolded instructions or by watching a screencast, a video recording of an expert
16
17 using the simulation. In both cases, students simultaneously answer supporting questions. The
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19 scaffolded instructions and supporting questions are designed to ensure that the students are
20
21 actively engaging in the learning task (Chi and Wylie, 2014) and focus students on identifying
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23 patterns in the data or observing how the particles interact to support them in developing an
24
25 understanding of the underlying concepts. The use of scaffolding and embedded assignment
26
27 questions to support students' use of simulations or screencasts is supported by Mayer's
28
29 cognitive load theory of multimedia learning (Mayer, 2011). By providing scaffolding and
30
31 questions to focus students on the most germane elements of the simulation and helping them
32
33 identify the patterns and/or make the connections required to build a conceptual understanding of
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35 a concept, we can reduce the cognitive load of the learning. Further, a recent study indicates that
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37 videos with embedded questions support learning better than reading from a textbook (Pulukuri
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39 and Abrams, 2021).
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49 When simulations or animations are used in class it is possible for the instructor to direct student
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51 attention to the more salient aspects of the animation or simulation. However, in such cases,
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53 students are limited in the amount of time they can spend observing the particle interactions and
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3 identifying patterns that can help them construct a coherent particle level understanding of a
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5 concept. As students enter our classrooms with very different backgrounds, it is reasonable to
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7 assume that they may require differing amounts of time watching or interacting with an
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9 animation or simulation to develop the desired mental model. When using such materials outside
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11 of class, students can spend as much time as they need interacting with the simulation or re-
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13 watching parts of the screencast (Keengwe and Kidd, 2010).
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19 We have previously reported that similar activities addressing other content areas where strong
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21 conceptual understanding requires accurate particle level models have resulted in significant
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23 learning gains with the screencast typically showing equal (Sweeder, Herrington and
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25 VandenPlas, 2019) or better results (Herrington, Sweeder and VandenPlas, 2017; Martinez *et al.*,
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27 2021; VandenPlas *et al.*, 2021). Since these activities are completed outside of class by the
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29 students, they also provide a common learning experience that the instructor can build upon in
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31 the classroom.
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38 *Learning During COVID Emergency Remote Instruction*

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40 The concern about learning loss as a result of COVID has been widespread. A recent study from
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42 the Netherlands suggests that the learning loss they saw was the equivalent of about one-fifth of
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44 a school year, with losses being up to 60% greater for students from less-educated homes
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46 (Engzell, Frey and Verhagen, 2021). Given the accessibility, physical, and emotional challenges
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48 that accompanied the disruption to education as instructors worldwide scrambled to learn new
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50 technologies and figure out how to move the teaching of classes and, in the case of chemistry,
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52 labs online, this learning loss is perhaps not surprising (DeKorver, Chaney and Herrington,
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3 2020). However, materials used during what many hoped would be a temporary move to remote
4 instruction, frequently focused on “moving content online.” The most frequently used strategies
5
6 were recorded lectures (asynchronous) or synchronous online lectures using platforms such as
7
8 Zoom, with some courses using small group breakout rooms, individual worksheets, and drop-in
9
10 virtual office hours (Gillis and Krull, 2020). Students generally reported a decrease in
11
12 instructional quality and learning as a result of the shift to remote instruction, though they also
13
14 reported preferring synchronous over asynchronous and classes that incorporated active learning
15
16 over just passive (Usher *et al.*, 2021). As the materials we describe in this paper were specifically
17
18 designed to support learning outside of a standard classroom setting, we felt it was important to
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20 compare results from students who completed these activities during a regular academic year to
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22 those from students who completed them during the spring 2021 semester when the course was
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24 taught online to determine whether difference existed in those two instructional environments.
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33 *Research Questions*

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35 Given the many challenges students have with the concept of equilibrium, combined with the
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37 challenges and affordances of the use of simulations and screencasts to support student learning
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39 of core chemistry concepts outside of the classroom, this study was guided by the following
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41 research questions:
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- 44 1. What differences exist between students who use the simulation on their own as
45 compared to those who view a narrated screencast of the simulation being used to
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47 investigate the concept of equilibrium?
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- 50 2. What are the major challenges students have in developing a particle level understanding
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52 of equilibrium?
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3. What learning differences are seen in the use of the developed simulation or screencast equilibrium materials to support in-person versus remote instruction?

Methods

Overview

The overall design and evaluation process used for this activity is outlined in Figure 1 and has been explained in detail for several other topics previously (Herrington, Sweeder and VandenPlas, 2017; Sweeder, Herrington and VandenPlas, 2019; Martinez *et al.*, 2021; VandenPlas *et al.*, 2021). A key element in this Backwards Design (Wiggins and McTighe, 2005) model is the use of student data to revise the assessments and activities. The following sections outline details of the activity design and evaluation process.

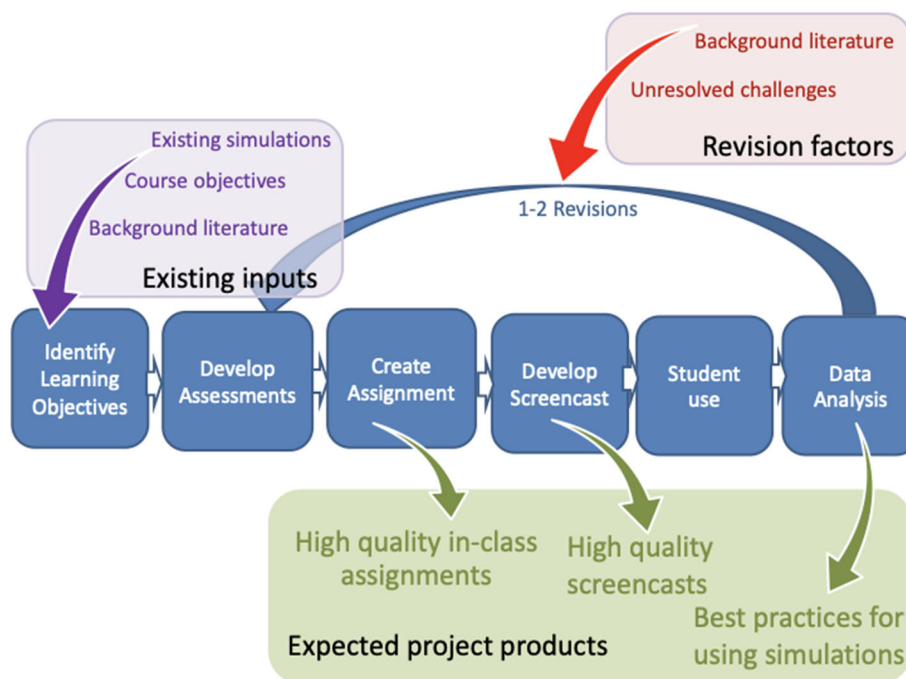


Figure 1: Outline of Activity Design and Evaluation Process

Assignment Design Process

All activities for the ChemSims project are designed to be introductory activities that focus on core chemistry concepts requiring an understanding of particle motion and interactions. Thus, it is important that we find a high-quality simulation to help students visualize the key particle motions and interactions and identify core course learning objectives that can be supported by interactions with and targeted observations of the simulations. We look for a simulation that:

1. accurately represents aspects of particle-level interactions (a challenge for many students);
2. focuses on common general chemistry learning objectives; and
3. provides a connection between the particle-level and some additional level of representation (e.g., graphical or macroscopic).

Making connections between representational levels is very important in developing a deep conceptual knowledge (Talanquer, 2011; Taber, 2013); however, this additional level of complexity makes it more difficult for students to make important connections on their own, thus necessitating quality scaffolding (Vygotsky, 1980). The identified PhET simulation (*Reactions & Rates*, no date) not only met these criteria, but was particularly attractive as it was used for the development of a related kinetics activity (Sweeder, Herrington and VandenPlas, 2019), which meant that many students had previously used this simulation to explore a different concept.

For equilibrium, the following learning objectives were identified.

Students should be able to:

1. Identify when a reaction reaches equilibrium by finding the point when the concentration of reactants and products remain relatively constant.

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- 2
- 3 2. Explain that equilibrium is a dynamic process. That the forward and reverse reactions are
- 4 constantly occurring, but that equilibrium occurs when those two rates are equal.
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- 8 3. Predict and explain how adding or removing reactants or products will influence the
- 9 equilibrium system to achieve a new equilibrium state by altering the rate of the forward
- 10 or reverse reactions.
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- 14
- 15 4. Describe how and why temperature affects the equilibrium position of endo- and
- 16 exothermic reactions differently.
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20 Before designing the activities, we identified suitable assessments that would allow students to
21 demonstrate if they had achieved the learning objective. These questions were used to create a
22 pretest and an analogous set of follow-up questions for the purpose of measuring student learning
23 gains (Table 1). These assessment questions guided how we would want students to interact with
24 the simulations and the observations that students would need to make to construct the desired
25 understanding. This provided the foundation for developing the scaffolded instructions and
26 questions embedded in the simulation assignment. We then used the simulation assignment as a
27 script for the screencast in which an instructor provided narrated interactions with the simulation
28 that students used to answer the same embedded assignment questions as the students who
29 interacted with the simulation on their own. Although the instructor helped to focus student
30 attention through their actions, they strove to avoid interpreting what the students were
31 observing, instead leaving students to do this as they answered the questions.
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50 **Data collection**

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52 This study was reviewed and approved as exempt by the Institutional Review Boards (GVSU ref.
53 No. 16-012-H; MSU x15-799e). All the participants voluntarily agreed to be in the study and
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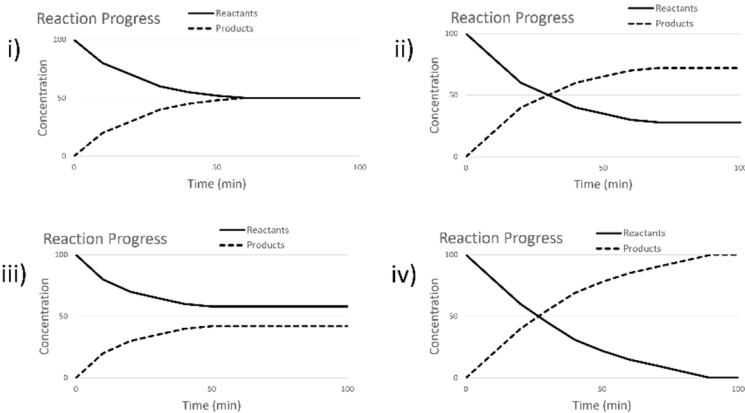
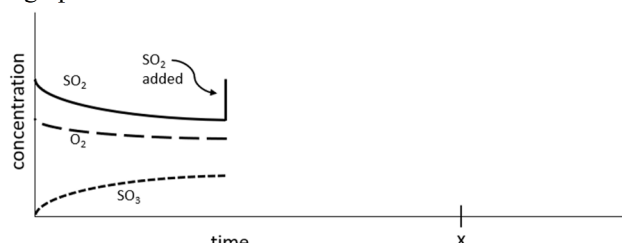
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3 consented through electronic forms to share their solutions and written thinking process on the
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5 assignments. During the 2021 data collect, one of the researchers was also one of several
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7 instructors simultaneously teaching the course. The activity was used as part of the standard
8
9 course instruction for all instructors and the researcher did not have access to information about
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11 consent until after the completion of the course. Data were collected from students enrolled in
12
13 second-semester introductory chemistry courses at two separate large public universities. At
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15 Institution 1, equilibrium is discussed after a focus on kinetics including collision theory,
16
17 reaction coordinate diagrams, rates of reactions and mechanisms. The introduction to kinetics
18
19 used a similar assignment based on the same PhET simulation, thus these students were already
20
21 familiar with the simulation. At Institution 2, equilibrium was discussed after acid and base
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23 chemistry and prior to kinetics and collision theory. Hence, to equip these students with
24
25 appropriate background knowledge, prior to completing the assignment, they all watched an
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27 additional 2-minute video that used the PhET simulation to introduce them to collision theory.
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29 Unlike the screencast assignment, this video did not require students to answer questions
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31 concurrent with their viewing and the narrator provided more interpretation of what was
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33 observed.
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42 Data were collected through several implementations. For all data collections, students
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44 completed a pretest and then their assignment outside of class prior to formal in-class discussion
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46 of the topic of equilibrium. However, the broad idea of equilibrium had been mentioned in
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48 previous relevant topics such as vapor pressure of liquids and colligative properties in solutions.
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50 For the initial data collection round ($N \approx 50$), analysis of student responses resulted in reworking
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52 some questions to better align the pretest and follow-up questions and ensure that the assignment
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3 prompts were effectively supporting students in their learning following the revision process
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5 outlined in Figure 1. The revised pretest and assignments were used in two subsequent semesters
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7 at the two different institutions (N=243 students), which again led to some additional minor
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9 revisions to address student learning challenges. This third version provides the basis for the pre-
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11 COVID data analysis used in this study and was deployed in five classes at the two institutions
12
13 (Table 2). This data collection was completed just before the institutions halted in-person classes
14
15 as a result of the COVID-19 pandemic. All students completed the pretest in class and then
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17 completed the assignment (screencast or simulation) including the embedded assignment and
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19 follow-up questions outside of class (for full assignment see Appendix A).
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26 The change to remote instruction for Spring 2021 provided an opportunity to directly compare
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28 the use of these materials to support in-person versus remote instruction. To do this, the
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30 screencast assignment was converted to an online-only format (*Version 4*) using Google Forms
31
32 (2018). Although we could keep most of the questions nearly identical in this different format,
33
34 one of the pretest and follow-up questions (Question 3 in Table 1) had to be modified. Since
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36 collecting images of drawings online had resulted in lower levels of participation in other studies
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38 (Sweeder and Herrington, 2020), we modified the question to have students select which graph
39
40 illustrated how the concentrations of species would change over time, and then provide an
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42 explanation as to why they chose that graph. The multiple-choice options were derived from the
43
44 most commonly drawn student responses for the paper and pencil version of the assessment. This
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46 implementation happened at a single institution across three classes (Table 2). Pre and posttest
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48 questions, along with how they were scored for pre-post analysis, are shown in Table 1. Full
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50 details of the scoring rubric can be found in Appendix B.
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Table 1: Pre and posttest questions

Question #		Scoring	Learning Objective
1	<p>Each graph below represents a reaction that involves the conversion of reactants to products and shows the concentration of each over time. Many reactions reach a state of equilibrium where there are some reactants and some products present in the reaction mixture.</p>  <p>a) Circle all of the graphs below that represent a system that comes to equilibrium. b) What features of the graphs indicated that the system was at equilibrium? c) For any graph that you circled above (meaning it reaches equilibrium), put a vertical line on the graph indicating the time point at which equilibrium was achieved.</p>	1 point total, $\frac{1}{3}$ point for each part a-c	1
2	<p>Your friends are discussing what they think they learned about why the concentrations of the reactants and products remain constant when a reaction reaches equilibrium.</p> <p>Betty: Because the concentration of the reactants is equal to the concentration of the products. Bob: Because the reaction stops before it reacts completely. Beth: Because the rate of reactants going to products is equal to the rate of products going back to reactants.</p> <p>a) Which friend do you think is correct? b) Explain why you think your other two friends are incorrect:</p>	1 pt each for explain why Bob and Betty were wrong	2
3	<p>The following reaction will reach an equilibrium.</p> $2\text{SO}_2 + \text{O}_2 \rightleftharpoons 2\text{SO}_3$ <p>If, while this system was at equilibrium, more $\text{SO}_2(\text{g})$ were added to the system, the concentration of SO_2 would initially increase as illustrated on the graph below.</p> 	Original 1 pt for correct drawing Revised: 1 pt for correct selection and correct reasoning	3

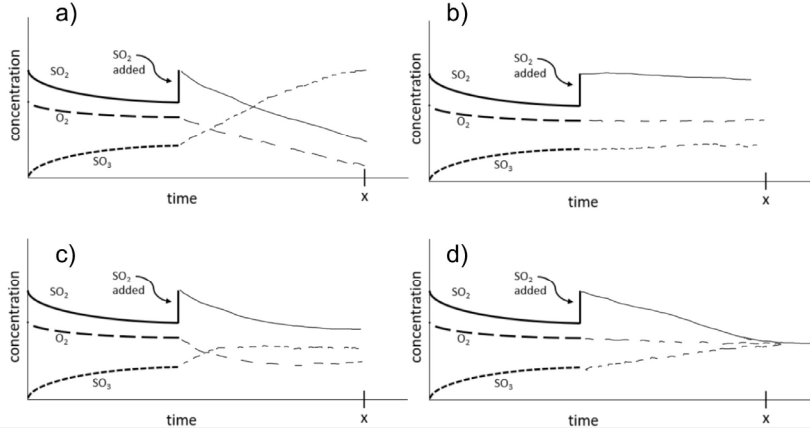
	<p>Original: Extend the concentration lines for each of the 3 compounds to timepoint x to illustrate how the concentrations of each would change as the reaction progressed.</p> <p>Revised:</p> <p>a) Which graph correctly shows what the concentration lines for each of the 3 compounds will look like as the reaction proceeds to time point x?</p>  <p>b) Explain why you chose the answer you did to the question above.</p>								
4	<p>This reaction of $N_2 + 3H_2 \rightleftharpoons 2NH_3$ is exothermic. What would you expect to happen to the amount of each compound present if, once at equilibrium, the temperature was decreased?</p> <table border="1" data-bbox="329 1010 1146 1255"> <tr> <td>N_2</td> <td>Increase / decrease / remain unchanged / impossible to determine</td> </tr> <tr> <td>H_2</td> <td>Increase / decrease / remain unchanged / impossible to determine</td> </tr> <tr> <td>NH_3</td> <td>Increase / decrease / remain unchanged / impossible to determine</td> </tr> </table>	N_2	Increase / decrease / remain unchanged / impossible to determine	H_2	Increase / decrease / remain unchanged / impossible to determine	NH_3	Increase / decrease / remain unchanged / impossible to determine	1 point if all changes were correct	4
N_2	Increase / decrease / remain unchanged / impossible to determine								
H_2	Increase / decrease / remain unchanged / impossible to determine								
NH_3	Increase / decrease / remain unchanged / impossible to determine								

Table 2: Summary of implementations

Version	Semester	Implementation	N (institutions/ classes/ students*)
3	Spring 2020	Pencil and paper; Simulation and Screencast	2 / 5 / 337
4	Spring 2021	Online data collection via Google Forms; Screencast only; Revised Question 3 (Table 1)	1 / 3 / 215

* For students the number represents those who provided consent for use of their data for research purposes and fully completed both the pretest and assignment activities.

Data analysis

Student Learning Gains

Student learning gains, as measured by pre and posttest questions, were determined using SPSS (*IBM SPSS Statistics 25*, 2017) to perform several statistical analyses. For the pre-COVID comparison of student performance using the screencast vs. the simulation assignment, a mixed 2-way ANOVA, with treatment (screencast or simulation assignment) as the between subjects variable and time (pre to post) as the within subjects variable, was used to compare overall changes in scores as well as to examine performance on each individual question. To measure learning gains for the COVID administration, we used paired sample *t*-tests, as there was only one treatment, the screencast. Finally, comparison of student gains between the pre-COVID and COVID administrations of the screencast assignment was done using a 2-way mixed ANOVA with year as the between subjects and time as the within subjects variables.

Student Particulate Level Understanding of Equilibrium

A major intent for the development of these activities was to help students construct a particle level understanding of equilibrium systems. We investigated student understanding by qualitatively analyzing student responses to particle level assignment questions that were separate from the pre and post assessment questions. The specific set of questions we analyzed for our qualitative analysis were:

- I. Starting the simulation reaction with the numbers of reactant and product particles shown below (specific starting number of particles for each reactant and product species provided):

- 1
2
3 a. At the beginning of the experiment, is the rate of the forward reaction (forming products)
4 faster / slower / the same as (circle one) the rate of the reverse reaction (forming
5 reactants)? What evidence from the simulation supports your conclusion?
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10 b. Use particle collisions (collision theory) to explain why the rates of the forward and
11 reverse reaction would initially be different.
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14 c. In general, after the reaction has occurred for a while, is the rate of the forward reaction
15 faster than / slower than / the same as (circle one) the rate of reverse reaction?
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19 d. Explain why this relationship between the forward and reverse reactions would make
20 sense based on the idea of Collision Theory and concentrations of products and reactants.
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24 For this set of questions, we first looked at whether students could correctly answer part a, which
25 in all cases was at least 70% of the students. If correct, we then coded their responses to the
26 subsequent questions. Open qualitative coding of these responses indicated answers fell into one
27 of three general categories: (i) correct use of particle collisions to explain relative rates; (ii) used
28 particle collisions, but did not explain relative rates; (iii) did not use particle collisions to explain
29 relative rates.
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40 Additionally, several questions were asked where students had to observe or predict what would
41 happen to the concentrations of reactants and products (increase/decrease/stay the same) in an
42 equilibrium system when a stress such as adding/removing a substance or changing temperature
43 was applied. For these questions we identified if students provided answer sets that were
44 internally consistent with reactions at a particulate level. For example, if students have a particle
45 level understanding of a chemical equilibrium, then they should understand that it is impossible
46 for the concentrations of *both* the reactants and products to increase if the temperature changes.
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3 For both the 2020 and 2021 data we looked at consistency for responses to question 4 on the
4 pre/post-test (Table 1) and three of the assignment questions that required similar reasoning.
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6 Additionally, in moving to the all online administration of the assignment in 2021, we revised
7
8 the question shown below from one that was more open (which side of the reaction will show an
9
10 increase in the number of molecules when we decrease the temperature? – and students write in
11
12 an answer) to one that forced student choices to (increased/decreased/stayed the same). This gave
13
14 us an additional two questions for comparisons of consistency in the 2021 data (shown below as
15
16 question II).
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21 II. Based on your observations from the simulation, after lowering the temperature and
22
23 allowing the molecules to reach a relatively stable distribution again, note what happens
24
25 to the concentration of the reactants and products:
26
27

28 a. For an endothermic reaction?

29
30 i. Reactant concentrations (increased/decreased/stayed the same)

31
32 ii. Product concentrations (increased/decreased/stayed the same)

33
34 b. For an exothermic reaction?

35
36 i. Reactant concentrations (increased/decreased/stayed the same)

37
38 ii. Product concentrations (increased/decreased/stayed the same)

39
40 c. How does Collision Theory help explain your answers to parts a and b?
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44 As part c to question II above also asked student for a particle level explanation, we initially tried
45
46 to qualitatively code student responses to this question as we had above with question I;
47
48 however, few students made the connection to activation energy and instead most attempted
49
50 explanations focusing on temperature impacting the kinetic energy of the particles or the
51
52 connection of energy associated with bond breaking and forming.
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Results

Student Learning Gains

2020 Simulation vs. Screencast analysis (pre-COVID)

An initial analysis for Institution 1 showed no differences based on instructor, so we were able to group students by treatment. Looking at overall student gains for each institution separately, for Institution 1 we see a main effect for time (pre to post) with an increase from 1.31 to 2.81 on a 5-point scale and a large effect size ($p < 0.001$, $F_{1,245} = 375.353$, $\eta_p^2 = .605$) as well as an interaction effect between time and treatment, albeit it with a small effect size ($p = .008$, $F_{1,245} = 7.187$, $\eta_p^2 = 0.028$). Figure 2 shows in this case the simulation students make slightly larger gains than the screencast students even though they started at a lower level. For institution 2 we see a main effect for time with an increase from 1.09 to 2.83 with a large effect size ($p < .001$, $F_{1,80} = 133.385$, $\eta_p^2 = .625$), but no interaction effect. As shown in Figure 2, in this case the screencast students make slightly larger gains than the simulation students, but the differences are not statistically significant. When all students from both institutions are combined, we found a significant main effect with respect to time for all students with a 1.55 point increase from 1.26 to 2.81 and a large effect size ($p < 0.001$, $F_{1,328} = 506.171$, $\eta_p^2 = 0.607$). However, there was no main effect for treatment or an interaction effect between treatment and time. Figure 2 also illustrates that the treatment resulted in a narrowing of the variance in scores between treatment groups, suggesting that students are as a whole at a more consistent level of understanding after completing the assignment, an effect that we have noted for another content topic (VandenPlas *et al.*, 2021).

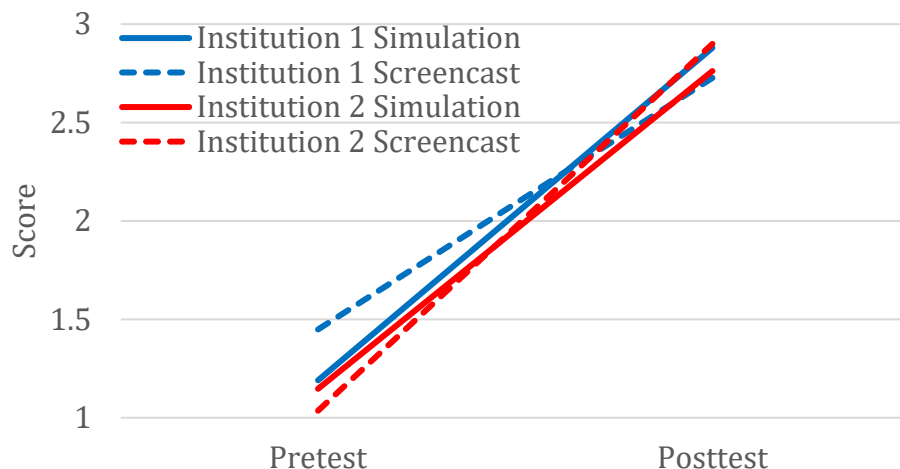


Figure 2: Pre to Posttest Change for Each Institution and Treatment

2020 vs. 2021 Screencast Comparison

Obviously, many changes occurred during the shift to remote instruction that go well beyond this assignment; however, the comparison between these implementations provides insight into the functioning of these assignments as instructional support tools in different learning environments. As this activity was only used at one of the institutions and it was only the screencast version that was used, the 2020 data used for comparison were the screencasts students from Institution 1. Further, because Question 3 had to be modified for the online administration and we were reluctant to use the score from this question to compare between years, we created a new total score, combining the results across Questions 1, 2, and 4 (out of a total of four points), for comparison purposes. Using a mixed 2-way ANOVA with year as the between subject variable, we saw an overall improvement from 1.27 to 2.36 with a large effect size ($F_{1,327} = 214.859$, $p = <0.001$, $\eta_p^2 = .397$) for the main effect of time. There was also a significant, but small interaction effect for the year ($F_{1,327} = 10.194$, $p = .002$, $\eta_p^2 = .030$) with the 2020 students showing a greater improvement from 1.12 to 2.54 compared to the 2021 students improving from 1.35 to 2.27.

2021 Revised Question 3 Analysis

Question 3 required significant changes in format as described above. In 2021, students were asked to select the correct graph that depicted how concentrations would change after the addition of a reactant to a system already in equilibrium and then explain their reasoning. Table 3 shows the distribution of graphical selections for students for each the pre- and posttest versions. The students' reasoning for selection of the graph was determined to be correct if they selected the correct graph and gave a reason that correctly invoked either correct initial changes to the concentrations *or* the reestablishment of a constant concentrations.

Table 3: 2021 2021 Student responses to revised question three

Graph Selected	Pretest % selected (correct reasoning)	Posttest % selected (correct reasoning)
a	20	22
b	14	14
c (correct)	34 (17)	44 (28)
d	32	20

Student Particle Level Understanding of Equilibrium

Student responses to several assignment questions were qualitatively coded to determine if the student used particulate level reasoning. For question I in the Data Analysis section, we looked at student explanations/evidence in parts a, b, and/or d because different students used particle collisions to answer different parts. Answers in part a or b indicating that initially there are more particles of reactants able to collide which makes the forward reaction faster, or in part d that after a while as products are formed they will collide and react so the rates will be equal were considered to have a *correct use of collisions*. If students wrote an answer like “particles will collide more” or “particles need to collide to react” in their explanations but did not connect it to the relative rates in any of the parts, then they were classified as *used particle collisions*, but that

they did not use the collisions to explain rates. The students that were classified as *not using particle collisions* most frequently gave answers that tried to use energy, talked about concentration in general but not about numbers of particles or collisions, or said that collisions had to occur with proper orientation and energy (basically just a statement of collision theory) but did not go any further. The frequency counts for each type of explanation for the different groups of students in this study are found in Table 4 below. Although we found all of these types of answers in all the different groups of students, the students from Institution 1 had a larger percentage of students in each case (simulation and screencast treatment and 2021 administration) who correctly used collisions to explain relative rates and had fewer students who did not use collisions at all.

Table 4: Student responses to Question I

Institution – Treatment	1 – Sim	1 - Screencast	2 - Sim	2 - Screencast	1 - 2021
Total number of students	62	94	46	45	214
Correct answer to part a (%)	89	70	78	71	81
(i) Correct use of collisions	54	68	36	44	54
(ii) Use of collisions	20	6	17	19	31
(iii) No use of collisions	25	26	47	38	15

To determine if student answers maintained internal consistency at a particulate level when considering the response of an equilibrium system to stress we examined six different questions. Each question required the students to observe or predict what would happen to the concentrations of reactants and products (increase/decrease/stay the same) in a given equilibrium system when a stress such as adding/removing a substance or changing temperature was applied. If students have a particle level understanding of chemical processes, their answers should always reflect that if reactants are consumed by a reaction, that the quantity of products should increase or vice versa. Any answer where students claim *both* the reactants and products increase

is not possible. For each of the (up to) six different question sets of this predictive format that the students encountered across the pretest, assignment, and follow up questions, we checked the set of student response for internal consistency. In any case where the question indicated that one specific compound was changed, we excluded the student response about that specific compound. For example, if compound A was removed from an equilibrium system, we ignored any response about the concentration of A. This is because it may not be clear if the students were considering the final equilibrium relative to the initial state or if the students is considering the final equilibrium relative to the moment immediately after the A was removed from the system. This meant that for some questions, students had to provide consistent answers across three question parts, whereas some questions looked at reactants or products as a set, so only two question parts were required to be consistent. These data are summarized below in Table 5.

Table 5: Consistency across questions

Question (# of question parts to be consistent)	Provided chemical viable answer	
	2020 (all students) N=149	2021 N=214
Pretest 4 – endothermic rxn (3)	68%	57%
Assignment – Predict (add product) (3)	78%	68%
Assignment – Predict (remove reactant) (3)	68%	60%
Assignment – Observe (cool endothermic rxn) (2)	*	90%
Assignment – Observe (cool exothermic rxn) (2)	*	85%
Posttest 4 – exothermic rxn (3)	83%	77%

*questions were not asked with forced responses so data is inconsistent

Discussion

Research Question One: Comparison of Student Outcomes with Simulation vs. Screencast

Research question one seeks to better understand any differences in learning that result between student use of the screencast as compared with the simulation to complete the out-of-class

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3 activity. The comparisons above in the results section (Figure 2) highlight that regardless of
4
5 institution or treatment, students generally made very similar learning gains with large effect
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7 size, and that the variance in scores at the class level was smaller with the posttest measurement
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9 than with the pretest. Further, the small effect size that was observed for differences between
10
11 treatments (screencast vs. simulation) at Institution 1 during the 2020 year, appears to have
12
13 arisen primarily due to the initial differences on the pretest scores, as the pretest scores between
14
15 the two treatment groups were statistically different while the posttest scores were equivalent
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17 between the two different treatment groups. These result are consistent with a previous study
18
19 using similar types of activities to introduce students to the topic of atomic interactions, which
20
21 also showed that the posttest learning outcomes were consistent across multiple classes,
22
23 regardless of differences in their pretest scores (VandenPlas *et al.*, 2021). Further, though we
24
25 have seen interaction effects with one treatment (simulation or screencast) making larger gains,
26
27 the effect sizes for these have always been small (Herrington, Sweeder and VandenPlas, 2017;
28
29 VandenPlas *et al.*, 2021). Finally, comparing the scores on the three nearly identical questions
30
31 between the in-person and online versions of the course also showed fairly consistent results.
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33 Together, these provide relatively good evidence that these learning activities can act as a solid
34
35 preclass introduction to equilibrium across a variety of class designs. Also, in general, having the
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37 students manipulate the simulation themselves or watch a narrated screencast will yield the same
38
39 overall outcomes. However, though not leveraged in this case, screencasts can provide an
40
41 opportunity for instructors to enhance the simulation experience, for example by allowing
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43 students to see side by side representations of two different conditions or by adding additional
44
45 non-simulation-based content, which may enhance student conceptual understanding
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3 (VandenPlas *et al.*, 2021). Further, the use of screencasts may circumvent student technology
4 issues for simulations that require software such as Java.
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10 *Research Question Two: Challenges in Developing a Particle Level Understanding of*
11 *Equilibrium*
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14 In many ways, research question two is the more interesting question. Although, pre-post
15 comparisons show learning gains. to determine how this activity affects students' particle level
16 understanding of equilibrium requires a qualitative look at student responses to questions that
17 offered them an opportunity to demonstrate particle level reasoning. From this, we gathered three
18 interesting takeaways.
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28 First, instructional content order can influence student learning. Our data suggest that
29 meaningfully learning about collision theory prior to engaging with the activity notably increased
30 students' ability to explain shifts in equilibrium using particle level reasoning. Student responses
31 to question I (Table 4), show that many of the students were able to correctly use Collision
32 Theory and the number of collisions to explain the relative rates of the forward and reverse
33 reactions with 36-68% of any class giving a correct explanation. However, what is striking about
34 these data is the disparity in the rates between the two different institutions. Here there is a
35 statistically significant difference between the two groups (58% vs. 40% correct, $z = 1.74$, $p =$
36 .041). We hypothesize that this difference arises from a difference in the order of content
37 between the courses at the two institutions. At Institution 1, kinetics and collision theory are
38 introduced prior to this activity involving equilibrium. However, at Institution 2, kinetics and
39 collision theory are encountered in more depth after equilibrium. Recognizing this difference and
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3 the need for students to use collision theory to explain equilibrium at the particle level, when the
4 activity was administered at Institution 2 we included a short introductory video and a few
5 related questions on collision theory, focusing on the fact that reactions occur as a result of
6 particle collisions. Unsurprisingly, we see statistically higher rates of the correct use of collisions
7 in explanations by students at Institution 1 who (presumably) had more comfort with that content
8 having learned and used it previously in the context of explaining kinetics concepts. Ensuring
9 that collision theory is deeply addressed prior to equilibrium may be key in addressing a reliance
10 on Le Chatelier's Principle for explaining equilibrium (Cheung, 2009) by ensuring that they have
11 the potential to construct a particle level explanation.
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26 The second takeaway was that many 2nd semester general chemistry students do not inherently
27 consider the consistency of sets of related answers when it comes to mass balance and chemical
28 reactions. A particle level understanding of chemical reactions and the Law of Conservation of
29 Mass necessitates that as an equilibrium system responds to a stress, either reactants are
30 increased and products decreased, or vice versa. Yet, as is evidenced by our data, internal
31 consistency of their answers is not yet an automatic consideration for all second semester general
32 chemistry students. In looking at their answers to a number of different questions that involved
33 disturbing systems at equilibrium and predicting or observing the changes to all the species
34 present (Table 5), 10-40% of students provided chemically impossible answers such as
35 suggesting that when one reactant was removed from a system, the concentration of one of the
36 products increased and the other decreased (a mass balance impossibility). In general, when
37 asked to describe what happened to reactants or products as a whole when a stress was applied
38 (e.g., what happened to the concentration of the reactants when the temperature was increased),
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3 students provided a chemically viable answer 85-90% of the time, meaning they recognized that
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5 as one went up the other had to go down. However, when asked to predict what would happen to
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7 individual reactant and product species when a given stress was applied, this number dropped to
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10 60-80% of students providing chemically viable answers. It should also be noted that the 2021
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12 students performed somewhat lower than the 2020 students on all of these questions (Table 5).
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17 The last takeaway was that it was extremely challenging for students to make the jump to use
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19 Collision Theory and particle motion to understand why a change in temperature would
20
21 differentially impact rates of forward and reverse reactions (question II part c). To correctly
22
23 apply Collision Theory to this phenomenon, students would have to recall and connect to
24
25 previous learning about activation energy and how that differs for exo vs endothermic reactions.
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28 Though this is something that is depicted graphically in the simulation, the activation of these
29
30 prior mental resources when learning a new topic is very challenging, even with suitable
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32 prompts. Though we tried to qualitatively code the student responses to this question, too few of
33
34 them gave answers that could be meaningfully grouped together. However, even if students are
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36 not yet able to make this connection on their own, the asking of the question can help students
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38 realize there should be a connection and help them identify where there might be a gap in their
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40 understanding so that instructors can more thoroughly engage with the topic during the follow-up
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42 class discussion.
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49 *Research Question Three: Supporting Student Learning for In-person vs. Online Instruction*

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51 As mentioned previously, the COVID-19 pandemic provided us with an opportunity to compare
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53 student outcomes when completing this activity as a supplement to an in-person, face-to-face
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3 class, as compared with those completing it as an activity that was part of a class offered online.

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5 Both classes regularly engaged students in group active learning activities during synchronous
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7 class meetings, with the online class using Zoom breakout rooms for group activities.
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10 Additionally, in both cases equilibrium screencast activities were completed by students outside
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12 of class as an introduction to the topic of equilibrium. One key difference between the two class
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14 formats was that the online class students were expected to complete a preclass activity on their
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16 own outside of class before attending each synchronous session. In the in-person class, these
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18 preclass activities were the exception as opposed to the norm.
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24 As reported in the Results section under *2020 vs 2021 Screencast Comparison* we saw both
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26 groups make significant gains from pre to post with a large effect size. Though we saw a small
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28 interaction effect for year with the 2020 students making slightly larger gains, given all of the
29
30 additional challenges that many students faced during the 2020-21 academic year, similar gains
31
32 could definitely be considered a success. Perhaps the largest take away from this comparative
33
34 analysis is the importance of question format on what can be gleaned from student responses. Of
35
36 particular note was Question 3 (Table 1). This question had to be substantially revised for use as
37
38 an online assessment question. Further, although we were able to generally classify student
39
40 drawing from the 2020 data into four main categories (represented by the four answer choices
41
42 shown in Table 1), coding individual student graphs was often quite challenging with respect to
43
44 determining which of two categories it should fit into. This may not be surprising as the ability to
45
46 draw and interpret graphs is an additional significant barrier for many students (Potgieter,
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48 Harding and Engelbrecht, 2008). With the initial question, the implicit assumption was that if
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50 students could correctly complete the lines on the graph that indicated they had a strong
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3 understanding of equilibrium as a dynamic system and the underlying basis for Le Chatalier's
4 Principle. In just asking students to choose the correct graph, we felt we needed to ask students
5 to explain their choice to determine how their understanding of equilibrium was involved in their
6 choice. Requiring this explanation was fortuitous as student responses provided some additional
7 insights into how students may have been approaching their drawings in 2020.
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17 *A complete* explanation of the correct answer would include both how the concentrations will
18 initially change after the addition of a reactant and that a new set of stable concentrations would
19 be formed. However, only 10% of the 2021 students on the post assessment included both of
20 these aspects in their explanation. More tended to provide an explanation that focused on only
21 the immediate change after the addition of the excess reactant, or on the fact that the
22 concentrations reached a “steady state”; however, each of these reasonings individually are
23 consistent with two different graph options. Interestingly, students who provided a pretest answer
24 that focused on the end state (stable concentrations) were more likely on the posttest to give an
25 answer that focused only on the changes immediately after the addition of the new compound
26 than to add this aspect to their already solid answer. This may suggest that the assignment
27 focuses students more on the initial changes, and not as much on the long-term equilibrium state.
28 This might also be explained by students' tendency to use one-reason decision making
29 (Talanquer, 2014), or it may be the case that the prompt did not provide enough structure to help
30 students understand that a complete explanation required addressing the initial change as well as
31 the final state (Cooper, Kouyoumdjian and Underwood, 2016).
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51 The incorrect explanations were also quite illuminating. Students who selected Graph a) (Table
52 3) correctly identified how the concentrations of compounds would shift after the disruption of
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3 the equilibrium but lacked the recognition that a new equilibrium would be reestablished. About
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5 a third of the explanations from these students suggested the students were simply applying Le
6
7 Chatelier's Principle as an algorithm. Students selecting Graph b) believed that the system at
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9 equilibrium would just remain at equilibrium or that no change would occur. This selection was
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11 generally accompanied by explanations that indicated students thought that no more reaction
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13 would occur after equilibrium was reached or that they were just focusing on the constant
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15 concentration part of the graph. Students selecting Graph d) primarily justified their selection
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17 with the idea that the concentrations of the compounds had to be equal to be in equilibrium.
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19 However, there were a few responses which seemed to indicate a misinterpretation of the graph
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21 such as "*The rates of each reaction whether forward or backward, became equal resulting in a*
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23 *conversion of each line.*" or "*all lines reach equilibrium as the concentrations and rxn rates are*
24
25 *equivalent. This means rate of rxn for fwd and rev rxns are =*". These students seem to recognize
26
27 the importance of the forward and reverse reaction rates being equal at equilibrium, but do not
28
29 fully understand equal rates does not necessarily mean equal concentrations. In this case they
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31 may be applying the and associative-activation heuristic where same means identical, rather than
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33 recognizing the same rates imply not equality with respect to concentrations, but rather
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35 unchanging (Talanquer, 2014).
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44 **Limitations**

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47 There are several limitations that should be noted when considering the results from this study.
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49 First, although we have seen equivalent results across institutions and instructors at two separate
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51 institutions, both institutions recruit students from similar backgrounds, and introductory
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53 chemistry courses at both institutions have course learning objectives that require students to
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3 provide particulate level explanations for chemical principles. Thus, differences may arise if
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5 these interventions were used with different student populations or in courses without an
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7 emphasis on particle level explanations. Second, though one of the benefits of students
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9 completing these activities outside of the classroom is that they are able to spend as much time
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11 engaging with the content as they need to, students must still choose to engage with the materials
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13 meaningfully. Requiring students to answer questions that focus them in on key aspects of the
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15 simulation, note patterns, and test their understanding throughout the activity helps support this
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17 meaningful engagement; however, it is likely that there are students who do not put in the time
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19 that they need, do not complete the activity in one sitting, or are distracted by other things while
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21 completing the activities. Lastly, the comparisons between the 2020 (in-person, pre COVID) and
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23 2021 (remote instruction) should be interpreted through the lens of the fact that the overall
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25 structure of the course and student experience changed dramatically. The online version
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27 employed far more preclass learning activities and a much greater role for group work and peer
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29 instruction during the class, at the same time many students were experiencing a great deal of
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31 fatigue with learning online.
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39 **Conclusions and Implications for Instruction**

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42 Equilibrium is a challenging topic for students; therefore, providing students with time to engage
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44 with the concept in a meaningful way on their own can serve as a productive common experience
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46 on which subsequent instruction can build. We have shown that both assignment formats
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48 (screencast or simulation) can serve as effective preclass experiences. Further, the detailed
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50 analysis of student responses to these assignments provides several insights that can help
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52 improve our instruction of equilibrium. First, the simulation appears to be most effective at
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3 helping students develop an appreciation of the dynamic nature of equilibrium, as the simulation
4 allows them to see and understand that the reaction itself proceeds in both a forward and reverse
5 direction. Second, the ability to develop a meaningful understanding of how dynamic
6 equilibrium relates to the direct interaction of particles, appears to be notably enhanced by the
7 students having meaningful prior experience with collision theory. This understanding is central
8 to explaining how equilibrium systems work and why they respond in a way that can be
9 predicted using Le Chatelier's Principle. As such, if we wish to move away from students overly
10 relying on Le Chatelier's Principle, then it would behoove us to ensure that the course content is
11 structured such that they have previously learned collision theory and thus have this as a
12 foundation for understanding equilibrium. Lastly, the student explanations for why they selected
13 different graphs highlights the need to focus instruction on both how the equilibrium responds to
14 the initial stress and the reestablishment of the equilibrium condition.

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33 The results from this study also provide some broader implications. The first is that this
34 intervention led to similar learning gains in similar populations of students regardless of
35 instructor, institution, or course modality. The consistency of the learning gains suggest that the
36 approach can be an effective initial introduction across a range of settings. However, as Eichler
37 (2022) suggests, this preclass activity should not be viewed as the entirety of instruction, but
38 rather just a foundation. If used effectively, such preclass activities can be used to inform
39 instruction and elicit student buy-in. Student responses can provide valuable insight into the
40 challenges that students are still having with the content so that in-class instruction can be short
41 and targeted so as to provide ample time for students to practice applying their understanding.
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54 This is consistent with findings by Bancroft et al. (2021) showing that in addition to pre and in-

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3 class activities with accountability, another required component for flipped instruction that
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5 resulted in significant gains in course GPA was the inclusion of responsive mini-lectures.
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7 Further, we have observed that sharing a summary of the students' responses to preclass
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9 activities at the start of class not only provides this targeted review of the content but also
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11 demonstrates to students the importance of the preclass activities for their learning and greatly
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13 increased their buy-in regarding the value of completing preclass activities.
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18 **Conflicts of Interest**

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21 There are no conflicts to declare.
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26 **Author Contributions**

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29 Sweeder and Herrington were involved in all aspects of study development and authorship of this
30
31 manuscript. Hilborn was involved with the formal analysis and the writing of the initial draft of
32
33 the manuscript. Sielaff was involved in the methodology and creating the initial assignment and
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35 early revisions.
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40 **Acknowledgements**

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42
43 The authors would like to thank Lauren Miling and Jessica VandenPlas for their assistance with
44
45 some of the early work on this study. Hilborn would like to thank Lyman Briggs College for
46
47 financial support. This material is based upon work supported by the National Science
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49 Foundation under Grant Nos. 1705365 and 1702592.
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Appendix A

Screencast Assignment (2020)

1) Go to the YouTube link <https://www.youtube.com/watch?v=cOZkwm3Es2s>, watch the introduction to reactions and rates and answer the following questions:

2) What is the current clock time?

3) Using the reaction where the A atom is yellow and the following initial conditions

$$A = 20 \quad BC = 15$$

$$AB = 1 \quad C = 0$$

a) How do the concentrations of reactants and products change initially?

b) How do they change after the reaction has occurred for a while?

c) The forward reaction and reverse reactions for this system are:



At the beginning of the experiment, is the rate of the forward reaction (forming products)

faster / slower / the same as (circle one) the rate of the reverse reaction (forming reactants)? What evidence from the simulation supports your conclusion?

d) Use particle collisions (collision theory) to explain why the rates of the forward and reverse reaction would initially be different?

e) In general, after the reaction has occurred for a while, is the rate of the forward reaction **faster than / slower than / the same as** (circle one) the rate of reverse reaction.

f) Explain why this relationship between the forward and reverse reactions would make sense based on the idea of Collision Theory and concentrations of products and reactants.

4) When 20 additional atoms of C are added:

a) In the table, predict what you think will happen to the number of each type of particle when the simulation is restarted and equilibrium is reestablished. Use Collision Theory and rates of the forward and reverse reaction to justify your predictions.

Particle	Predict: Increase/ Decrease	Justification of your predictions based on rates of forward and reverse reactions
A		
BC		

AB		
C		

- b) Was your prediction correct? Yes / No (circle one)
 c) If your prediction was not correct, explain what actually happened.

Try it Yourself

Go to the PhET simulation Reactions & Rates: <https://phet.colorado.edu/en/simulation/legacy/reactions-and-rates>. Note: You will need Java installed (see separate Java instructions). To start: Microsoft edge - click the image of the simulation; Chrome or other browsers you may have to download the simulation, then open it.

Set up the experiment as in the screencast with the following initial conditions:

$$A = 20 \quad BC = 15$$

$$AB = 1 \quad C = 0$$

- Bring up the strip chart. Zoom out on the strip chart so that you can see 20 molecules on the y axis.
- Adjust the initial temperature so that the total average energy line is halfway between the potential energy of the products and peak of the reaction coordinate diagram.
- Begin the experiment and allow it to run for a while and then pause the simulation

- d) What do you anticipate will happen to the number of each kind of particle if you **decrease** the number of one of the types of particles? Circle the type of particle you want to decrease the number of, and then as before, complete the table below.

Particle	Predict: Increase/ Decrease	Justification of your predictions based on rates of forward and reverse reactions
A		
BC		
AB		
C		

- e) Adjust the amount of the particle you circled above, and test your prediction. Was your prediction correct? Yes / No (circle one)
 f) If your prediction was not correct, explain what actually happened.

Going Further: Impact of temperature

- 5) Click End Experiment. When you click Begin Experiment, it should reset with the conditions from part 3.

Begin the experiment with the same settings and wait for the simulation to reach a relatively consistent number of each particle. Note the number of each particle type:

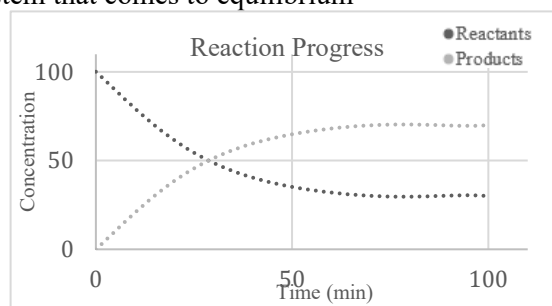
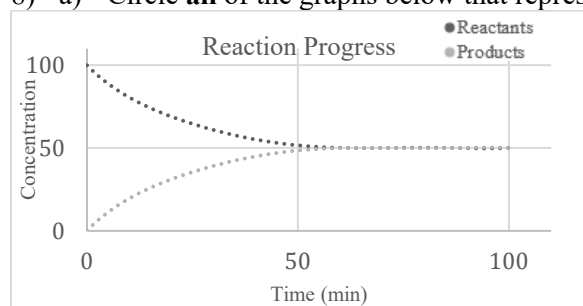
A = AB =

BC = C =

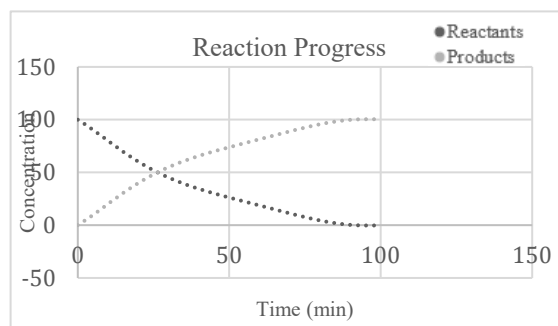
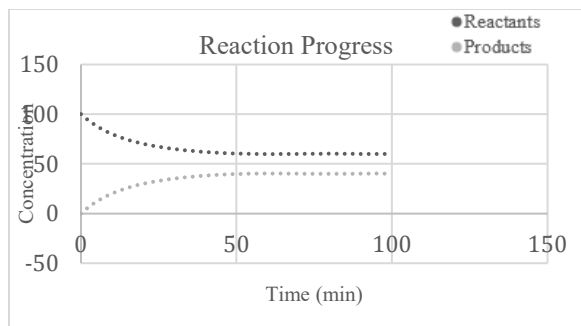
- a) Lower the temperature considerably. What happens to the total average energy as this happens?
- b) Allow the molecules to reach a relatively stable distribution again. Once this happens, are there more reactants, more products, or have each remained unchanged?
- 6) Switch the exothermic reaction (4th reaction with red atom of A). Begin the Experiment using the same setting used in part 5. (Note, the Total Average Energy line may not move when you do this.) As before, allow the number of molecules to stabilize and record the numbers.
- A = AB =
- BC = C =
- a) Lower the temperature considerably. What do you notice about the change in reactant and product molecules?
- 7) Looking at your results from parts 5 and 6, which side of the reaction will show an increase in the number of molecules when we decrease the temperature?
- a) Part 5 - endothermic?
- b) Part 6 - exothermic?
- c) How does Collision Theory help explain your answers to parts a and b?

Follow Up - Using your findings

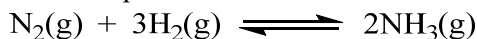
- 8) a) Circle **all** of the graphs below that represent a system that comes to equilibrium



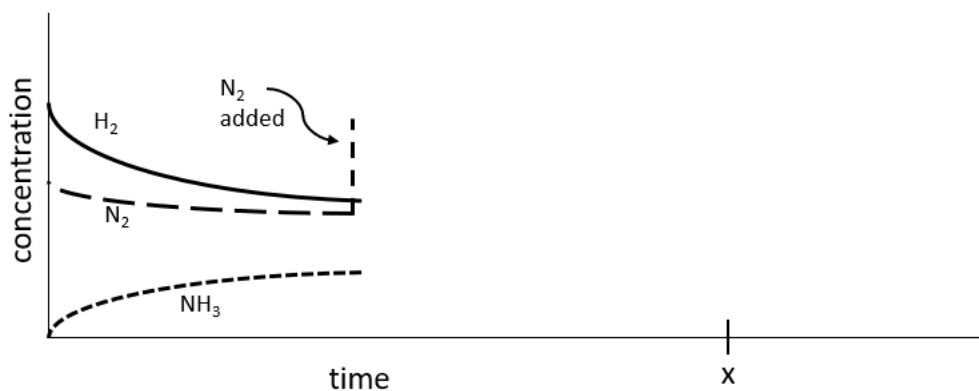
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- b) What features of the graphs indicated that the system was at equilibrium?
- c) For any graph that you circled above (meaning it reaches equilibrium), put a **vertical line** on the graph indicating the time point at which equilibrium was achieved.
- d) Your friend Bob says a reaction reaches equilibrium because the reaction stops. You know this is not correct. How would you explain to Bob why the concentrations remain constant at equilibrium?
- e) Your friend Betty says that at equilibrium means that the concentration of the reactants and products are equal. You know that is not correct. What would you tell Betty is actually equal at equilibrium?
- 9) The following reaction will reach an equilibrium.



If, while this system was at equilibrium, more $\text{N}_2(\text{g})$ were added to the system, the concentration of N_2 would initially increase as illustrated on the graph below. Extend the concentration lines for each of the 3 compounds to timepoint x to illustrate how the concentrations of each would change as the reaction progressed.



- 10) The reaction of $2\text{SO}_2 + \text{O}_2 \rightleftharpoons 2\text{SO}_3$ is exothermic. What would you expect to happen to the amount of each compound present if, once at equilibrium, the temperature was decreased?

$\text{SO}_2(\text{g})$	Increase / decrease / remain unchanged / impossible to determine
$\text{O}_2(\text{g})$	Increase / decrease / remain unchanged / impossible to determine

SO ₃ (g)	Increase / decrease / remain unchanged / impossible to determine
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Appendix B

Coding and scoring scheme used

Question	Coding Scheme	value
1a) selecting systems at equilibrium (Pre and posttest)	¼ credit for each correctly indicate (i, ii, and iii selected, iv not selected)	0.3333 total
	1 = concentrations constant/reactants and products are constant OR rates equal/constant OR graphs level out/straight parallel lines (correct)	0.3333
1b) why were 1a selected? (Pre and posttest)	2 = reactants and products are equal/have equal concentrations OR Graph lines meet or end at the same place	0
	3 = Meet at a point OR conc of reactants and products are equal at some point OR lines cross or meet	0
	4 = approach an intermediate value OR curves approach one another	0
	5 = other	0
1c) When is equilibrium established? (Pre and posttest)	1 = consistently selected where curves start to flatten out (correct) [this was still possible if iv was also selected in part 1a]	0.3333
	2 = Consistently selected where curves cross/meet	0
	3 = Inconsistent or other	0
2 Who was correct (not scored for points) (pretest only)	1 = Beth 2 = Betty 3 = Bob 4 = Other (e.g., circled more than one)	
2 Why was Bob wrong? (pretest and posttest)	1 = something about reactions continuing but rates being equal	1
	2 = reaction doesn't stop	0
	3 = concentration remains constant	0
	4 = something about the reaction not being at equilibrium if it goes to completion or reactant is used up	0
	5 = misc	0
	6 = reaction goes to completion	0
2 Why was Betty wrong? (pretest and posttest)	1 = something about it is the rates that are the same, not the concentrations OR that the concentrations remain constant but don't have to be equal	1
	2 = concentrations don't have to be equal to reach equilibrium	0
	3 = misc	0
2 Why was Betty wrong? (Pretest only)	1 = it is the rates that are the same, not the concentrations OR that the concentrations remain constant but don't have to be equal	Not scored
	2 = concentrations don't have to be equal to reach equilibrium	Not scored
	3 = misc	Not scored

3 selection (Pre and Post)	Coded by selection	
	1 = Indicates that initially SO ₂ and O ₂ should decrease while SO ₃ increases AND indicates that constant concentrations will be reestablished	1 point if correct graph selected
	2 = indicates that constant concentrations will be reestablished (focus only on ending state)	0.75 point if correct graph selected
3 Reasoning (Pre and post)	3 = Indicates that initially SO ₂ and O ₂ should decrease while SO ₃ increases or other Le Chatelier' Principle inspired statement (focus only on initial change after addition of SO ₂)	0.75 point if correct graph selected
	4 = just "reaches equilibrium" without indicating what that means or supporting w prod/reactants	0
	5 = other responses	0
4 (Pre and Post)	Coded by selections for N ₂ / H ₂ / NH ₃	
	Decrease /decrease / increase	1 (consistent)
	Increase / increase / decrease	0 (consistent)
	No change / No change / no change	0 (consistent)
	All other combinations	0 (inconsistent)

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