Shape Thinking: Covariational Reasoning in Chemical Kinetics

Jon-Marc G. Rodriguez Purdue University
Kinsey Bain Purdue University
Felix Ho Uppsala University
Marcy H. Towns Purdue University

This work addresses the following research question: In what ways do students use mathematics in combination with their knowledge of chemistry and chemical kinetics to interpret concentration versus time graphs? The study was designed and implemented using a resource-based model of cognition as the theoretical framework. Data was collected through the use of an assessment involving short-answer test items administered to 109 students in a first-year, non-majors chemistry course at a Swedish university. The student responses were translated from Swedish to English and subsequently coded. Data analysis involved using the shape thinking perspective of graphical reasoning as a methodological framework, which was adapted to analyze the covariational reasoning used by students in the context of chemical kinetics. Open-coding and considerations of shape reasoning have provided insight into student understanding of mathematical models of chemical processes.

Keywords: Graphing, Covariational Reasoning, Shape Thinking, Rates, Chemistry

Introduction and Rationale

Chemical kinetics is concerned with the rate of change of concentration of compounds in a chemical reaction, which readily lends itself to be described using differential calculus. Mathematical operations and graphical reasoning centered around the derivative provide useful tools for modeling systems that are changing over time. However, a review of the literature indicates students lack a clear understanding of rate and rate-related ideas, with ample evidence supporting the claim that students struggle with a conceptual understanding of functions, covariational reasoning, and assigning meaning to variables (Aydin, 2014; Bain & Towns, 2016; Castillo-Garsow, Johnson, & Moore, 2013; Moore, 2014; Moore, Paoletti, & Musgrave, 2013; Rasmussen, Marrongelle, & Borba, 2014; White & Mitchelmore, 1996).

Given this backdrop, it is not surprising students have difficulty using and applying calculus in other contexts, such as modeling physical systems (Becker & Towns, 2012). The act of modeling, in which processes are translated into mathematical formalism, is a common practice in the sciences, and it has been identified as a foundational scientific practice that students should engage in at all levels of education (Bruce, 2013; National Research Council, 2012; Edwards & Head, 2016; Posthuma-Adams, 2014). However, problem-solving, reasoning, and modeling in the physical sciences is particularly challenging because it introduces an additional domain of (scientific) knowledge that must be integrated with a student's mathematical knowledge, a problem that is further compounded when considering that chemistry requires students to think abstractly at the particulate-level, which is not readily observable or accessible (Becker & Towns, 2012). Nevertheless, researchers agree that making connections across different domains of knowledge through modeling is necessary to promote a deeper understanding of chemistry (Becker, Rupp, & Brandriet, 2017; Sjostrom & Talanquer, 2014; Taber, 2013; Talanquer, 2011).

Based on this rationale, research studies have investigated student understanding of mathematical expressions and their relationship to chemical phenomena, and published literature reviews indicate there have also been a number of other studies that focus specifically on chemical kinetics (Bain & Towns, 2016; Becker et al., 2017; Becker & Towns, 2012; Greenbowe & Meltzer, 2003; Hadfield & Wieman, 2010; Jasien & Oberem, 2002; Justi, 2002). In their review paper, Bain and Towns (2016) echo the call of the National Research Council for more discipline-based education research (DBER) that focuses on studies at the undergraduate level and emphasizes interdisciplinary work, such as collaborations between chemistry and mathematics communities. They also comment specifically on the need for more studies that incorporate prompts aimed at investigating graphical reasoning in a chemical context such as kinetics (Bain & Towns, 2016).

Among the reviewed literature, few studies focus on the overlap of chemical and graphical reasoning, and among the chemical kinetics studies reviewed, none focus exclusively on reasoning related to graphical representations. However, student difficulties with graphs are discussed briefly as part of larger studies and the general consensus among the literature is that students are often unable to make conclusions about the chemical mechanism that is implied in graphical representations of chemical processes (Cakmakci, 2010; Cakmakci & Aydogdu, 2011; Cakmakci, Leach, & Donnelly, 2006; Kolomuç & Tekin, 2011; Tastan, Yalçinkaya, & Boz, 2010). This study seeks to fill the gap in the literature and contribute to the body of knowledge related to graphical reasoning in the physical sciences. To this end, our guiding research question is the following: In what ways do students use mathematics in combination with their knowledge of chemistry and chemical kinetics to interpret concentration versus time graphs?

Theoretical Underpinnings

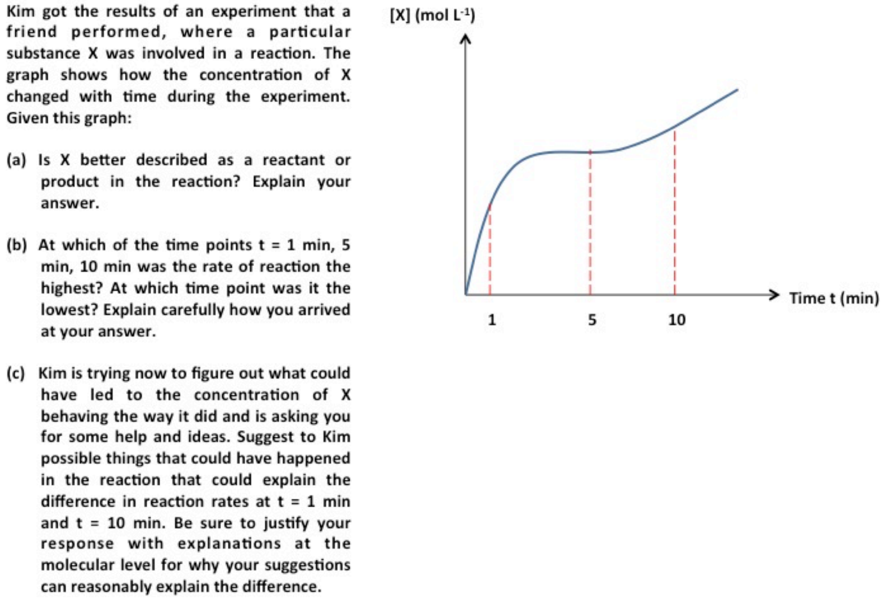
This study was developed using the resource-based model of cognition as a theoretical framework (Hammer & Elby, 2002, 2003). The resources perspective describes student knowledge as being defined by resources that are activated in specific contexts. These resources are broadly defined as pieces of knowledge or ideas about the nature of knowledge. Hammer and Elby (2002) emphasize that resources may be productive or unproductive, and instruction should focus on understanding what resources students have and how to encourage students to use resources that are useful for a given context. As mentioned by Becker and colleagues (2017), using the resources perspective to frame data analysis and dissemination of results provides the opportunity for researchers and practitioners to consider what instructional support would be useful to help students productively use their knowledge. By considering the nature of the student responses and the reasoning elicited from the prompt, appropriate scaffolding can be developed to encourage scientific reasoning and promote scientific practices such as modeling.

To aid in the analysis of our data, we used the shape thinking perspective as a methodological framework (Moore & Thompson, 2015). Within the shape thinking framework, reasoning related to graphical understanding and problem-solving is characterized as static or emergent: static thinking is reasoning that describes graphs as objects ("a wire") that have associated properties; emergent thinking is reasoning about graphs as a mapping of all of the possible inputs and outputs, a trace in progress (process) involving covarying quantities.

Methods

Data Collection

The primary source of data was an assessment administered to 109 students following the chemical kinetics unit in a first-year non-majors chemistry course at a Swedish university. The prompt given to the students provided a concentration vs. time graph along with three short-answer questions related to the graph (see Figure 1). One of the learning objectives for the kinetics unit involved getting students to extract information about what is happening at the molecular level from a graphical representation of a reaction. This is reflected in the design of the prompt, which focuses on conceptual understanding and requires students to integrate chemical and mathematical knowledge.



Kim got the results of an experiment that a friend performed, where a particular substance X was involved in a reaction. The graph shows how the concentration of X changed with time during the experiment. Given this graph:

(a) Is X better described as a reactant or product in the reaction? Explain your answer.

(b) At which of the time points t = 1 min, 5 min, 10 min was the rate of reaction the highest? At which time point was it the lowest? Explain carefully how you arrived at your answer.

(c) Kim is trying now to figure out what could have led to the concentration of X behaving the way it did and is asking you for some help and ideas. Suggest to Kim possible things that could have happened in the reaction that could explain the difference in reaction rates at t = 1 min and t = 10 min. Be sure to justify your response with explanations at the molecular level for why your suggestions can reasonably explain the difference.

Figure 1. Prompt used for assessment.

This emphasis on conceptual understanding led the researchers to consider ideas of transfer. Transfer involves applying knowledge to unfamiliar situations, and the ability to transfer knowledge has been identified as a key component of conceptual understanding (Holme, Luxford, & Brandriet, 2015). Within the resources framework, transfer is conceptualized as the *activation of resources*, and in order for students to be able to use knowledge in novel situations, resources related to the task need to be coherently organized in such a way that they are not dependent on a single context (Hammer, Elby, Scherr, & Redish, 2005).

The prompt was designed, in part, to evaluate the extent in which students are able to use the appropriate knowledge in a different context. The graph in the prompt did not reflect the concentration vs. time graphs normally depicted in textbooks, and although chemically possible, it exhibited deviations from empirical results one would observe in typical laboratory work done in a general chemistry course (see Figure 2). In addition to representing a somewhat unfamiliar problem-solving scenario, item (c) in the prompt reflects what is described as an “ill-defined” problem, in which the question is more open-ended and there is not just one correct answer (Singer, Nielson, & Schweingruber, 2012). For this problem students are prompted to suggest a plausible explanation for the observed graph shape, which could encompass a myriad of possible justifications. Content validity of the assessment items was achieved by discussing and co-developing this prompt among a group of four researchers, and the wording in the prompt was refined after initially being piloted (in both English and Swedish) with a group of participants that included three professors, a postdoctoral researcher, and two Ph.D. students.

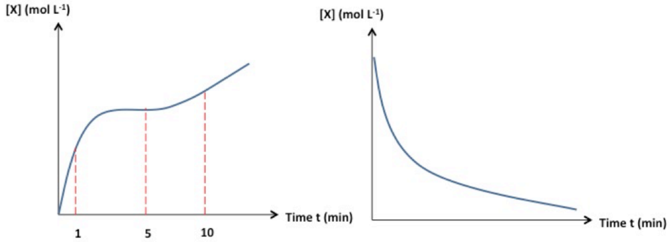


Figure 2. Graph used in the prompt (left) and a graph used in a typical chemistry textbook (right).

After translating the student responses from Swedish to English, they were analyzed using open coding and the shape reasoning framework. Through the process of constant-comparison a list of codes was created and refined, with a graduate student and a postdoctoral researcher coding in tandem and requiring 100% agreement for assignment of codes (Patton, 2002). The coding scheme developed into a multi-tier categorization system that was used to characterize student reasoning. The scheme characterizes the student responses, first based on whether the student answered the question correctly, then on the discipline-specific (chemistry vs. mathematics) resources, such as the content and reasoning the students used. This was developed through a combination of inductive and deductive analysis, in which the chemistry categories developed as a result of the observed student responses and the mathematical reasoning categories were modeled after the previously mentioned delineation of emergent vs. static reasoning in the shape thinking framework (Moore & Thompson, 2015). For the chemistry categories, a "Less Productive" sub-category was created to encompasses responses that involve ideas that are not useful for problem-solving in this context and/or reflect incorrect reasoning about relevant ideas, and a "Kinetics Concepts" sub-category was created to encompasses ideas and reasoning that more appropriately address the prompt. It is also important to note that chemical and mathematical reasoning categories are not mutually exclusive (e.g. a student response can employ both chemical and mathematical reasoning), and here the authors describe the development of a new construct called *process thinking*, which encompasses chemically plausible explanations and emergent reasoning, illustrating higher-level modeling that involves the productive use of cognitive resources (example to follow).

Preliminary Results

Analysis of the data reveals that students employ multiple different types and combinations of chemical and mathematical reasoning when interpreting concentration vs. time graphs.

When considering student responses to the first item on the assessment, (a), which asks the students to decide if the graph depicts changes in the amount of product or reactant, it can be seen that there was little variation in student reasoning; most students responded with the same chemically plausible idea that since reactants are consumed (decrease) and products are formed (increase) over the course of the reaction, the graph represents products increasing over time. In responding to this prompt, students also tended to consider how both variables change over time, displaying emergent reasoning. For the second assessment item, (b), which tests students' abilities in making connections between a graphical understanding of the derivative and ideas related to rate, the students tended to respond in purely mathematical terms without bringing in chemical knowledge, with most students reasoning statically, only thinking about the general shape and the steepness of slopes, rather than considering more formal definitions of the derivative. In the case of the final prompt, (c), which asks students to essentially trace the function and discuss the chemical phenomena that could explain the observed graph, most students responded in general terms, providing lists of factors that affect rate, rather than specifically considering the chemistry occurring at each point. However, a few students expressed a deeper level of understanding. Consider Eleanor's response to (c):

> We can see from the graph that from t = 0 to about t = 3, the rate of reaction increases, it means the concentration of reactants is greater than the concentration of products. Such a difference in concentration leads to the increase in the products' concentration. But when the reaction reaches t = 5 we can see that the product's concentration has stopped increasing, this means that the reaction has reached an equilibrium. That is why we do not get an increase in the concentration of X. But we see how at t = 7 the reaction will keep forming products. This is because we no longer have an equilibrium. And one way to change the equilibrium can for example be through changing the temperature in the reaction or through adding more reactants to the reaction so that they can continue to form products.

In her response, Eleanor considers multiple points on the graph and provides chemically plausible explanations that could justify the observed shape of the graph. Responding to item (c) requires mechanistic thinking about the process the graph models, and as instructors, we would like to move students toward a more sophisticated understanding that encompasses practices such as modeling, a level of reasoning (exemplified by Eleanor) that defines the construct we call *process thinking*. Process thinking combines chemically plausible explanations with emergent reasoning (mathematical reasoning related to functions and covariation), and preliminary results indicate process thinking was not common among the student responses. This does not necessarily imply students are unable to engage in this level of reasoning, because this prompt may not have been effective in activating or eliciting this type of reasoning.

Preliminary analysis also yielded some interesting considerations regarding language and culture. In Swedish, the standard mathematical term for the gradient of a line in two-dimensional space is *lutning*, which is the noun form of the verb *luta*, "to lean". Both words are of general, everyday usage, but are nevertheless used in Swedish to describe the characteristics of a line in the more specialized, mathematical context. Furthermore, this description of the derivative is dynamic in the way that it connotes action. For instance, from its grammatical construction, the word *lutning* is literally "leaning-ness" or the act of leaning. Also, a line can *luta skarpt*, "lean strongly", as opposed the more static description of a line *having* a steep gradient/slope, as is the norm in English. This suggests some level of cultural and colloquial familiarity or association for the students.

Conclusion and Questions

When viewing the student responses as variations in reasoning that reflect cognitive resources available to the students, it is worth evaluating which resources are more productive for the context, and investigating the extent in which each item in the assessment elicited the desired reasoning. This will provide a better understanding of how to scaffold student reasoning, promote modeling, and develop exams that can assess deeper levels of understanding. Further analysis is warranted and the following questions reflect potential future avenues for inquiry:

(1) How are the types of chemical and mathematical reasoning related for each response?
(2) How do we promote modeling and activate productive resources in unfamiliar situations?
(3) What role do cultural influences such as language have on student mathematical reasoning and our coding scheme?

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