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Complete List of Authors:	Bain, Kinsey; Purdue University, Chemistry Rodriguez, Jon-Marc; Purdue University, Chemistry Moon, Alena; University of Michigan, Chemistry Towns, Marcy; Purdue University, Chemistry

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ARTICLE

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Kinsey Bain,[a] Jon-Marc G. Rodriguez,[a] Alena Moon,[b] and Marcy H. Towns[a]

Chemical kinetics is a highly quantitative content area that involves the use of multiple mathematical representations to model processes and is a context that is under-investigated in the literature. This qualitative study explored undergraduate student inegration of chemistry and mathematics during problem solving in the context of chemical kinetics. Using semi-structured interviews, participants were asked to make their reasoning and thinking explict as they described provided equations and as they worked though chemical kinetics problems. Here we describe the results from our study, which included thirty-six general chemistry students, five physical chemistry students, and three chemical engineering students. Analysis and findings are framed in terms of blended processing, a theory from cognitive science that characterizes human knowledge integration. Themes emerged relating to contexts that were commonly discussed when blending occurred. Variation in the depth and directionality of blending was also observed and characterized. Results provide implications for supporting student problem solving and the modeling of chemical processes.

Introduction

Chemistry is often symbolized and discussed using variations of the "chemistry triplet", which identifies the different modes of representation and involves thinking at the macroscopic, particulate, and mathematical/symbolic levels (Johnstone, 1991; Mahaffy, 2004, 2006; Sjostrom and Talanquer, 2014; Taber, 2013; Talanquer, 2011). Although the limitations of this model have been identified and revisions have been suggested, the power of this model derives from its simplicity, and making connections between different levels of representation has been identified as a critical part of having a deep conceptual understanding of chemistry (Cooper et al., 2015; Holme, Luxford, and Brandriet, 2015). The process in which connections are made between different domains can be described as modeling. Although a formal description of a *model* is often dependent on the discipline and context, using modeling to describe student thinking is useful, because the different definitions of models share common features (Lesh and Doerr, 2013; Oh and Oh, 2011). Here, we describe (scientific) models as abstract representations of a system that have limitations and derive utility from their predictive and generative nature (Harrison and Treagust, 2000; Schwarz, Reiser, Acher, Kenyon, and Fortus, 2012; Schwarz et al., 2009). The act of modeling then becomes the process by which students use, evaluate, and construct models that are consistent with empirical data, encompassing what Schwarz et al. (2009) describe as *modeling metaknowledge*, which involves a working understanding about the nature of models (limitations, development from empirical evidence, dependence on context, etc.).

Research suggests that at the university-level, student models of scientific concepts are often underdeveloped and lack sophistication, even at the graduate-student level, indicating a need to embed models and model-building activities into the undergraduate curriculum (Bhattacharyya, 2006). Engaging students in modeling is critical because using scientific models and understanding their limitations, such as their provisional or context-dependent nature, is central to the basis of scientific knowledge (Taber 2010). However, according to Driver et al. (1994) clearly communicating these ideas and constructing scientific knowledge is not trivial:

"The challenge lies in fostering a critical perspective on scientific culture among students. To develop such a perspective, students will need to be aware of the varied purposes of scientific knowledge, its limitations, and the bases in which these claims are made."

Therefore, in order to better guide students on how to engage in modeling there is a need to characterize the cognitive processes involved in developing and using models. In this study, we utilized *blended processing* as a framework to describe the distinctive features of student engagement in modeling as they reason about mathematics and chemistry (Coulson and Oakley, 2000; Fauconnier and Turner, 1998).

This study is situated in the context of chemical kinetics because it is often framed as a highly quantitative topic and it is currently not well-represented across the literature (Bain and Towns, 2016; Becker, Rupp, and Brandriet, 2017; Justi, 2002). In addition, chemical kinetics is taught at multiple levels

[a.] Department of Chemistry, Purdue University, West Lafayette, Indiana, 47907, United States.
[b.] Department of Chemistry, University of Michigan, Ann Arbor, Michigan, 48109, United States.

of the undergraduate chemistry curriculum, and there is a need for discipline-based education research that moves beyond introductory-level courses (Singer, Nielson, and Schweingruber, 2012). To this end, this study addresses the following research question: *In what ways do chemistry and mathematics knowledge interact as students engage in chemical kinetics problem solving?*

Review of related literature

Mathematics and chemistry

The use of mathematics as a tool to understand the physical world – mathematical modeling – is essential to the study of chemistry. To understand chemistry concepts, students must be able to understand the mathematical symbols and operations and the physical meaning they represent (Becker and Towns, 2012). Because of this reality, some work in recent years has been done to investigate students' understanding and use of mathematics in scientific contexts. For example, there is much evidence that emphasizes the importance of mathematical understanding and ability for success in general and physical chemistry (Bain, Moon, Mack, and Towns, 2014; Derrick and Derrick, 2002; Hahn and Polik, 2004; House, 1995; Nicoll and Francisco, 2001; Spencer, 1996; Tsaparlis, 2007; Wagner, Sasser, and DiBiase, 2002). Others have investigated how students understand mathematical expressions. Becker and Towns (2012) found that most students could interpret total and partial differentials, as well as provide accurate physical meaning represented by the mathematical expressions. However, they did find that students had difficulty writing expressions or applying information from descriptions of physical situations, which is consistent with findings in physics education research where students could not connect the mathematics with physical scenarios (Thompson, Bucy, and Mountcastle, 2006; Bucy, Thompson, and Mountcastle, 2007),

Mathematics is often used in chemistry when understanding and solving problems. There is much research on quantitative problem solving in science education research, where studies typically look at students' abilities to solve the problem correctly (including rubric use and development) (e.g., Wilcox, Caballero, Rehn, and Pollock, 2013), to understand and set up the problem (e.g., Bodner and McMillen, 1986), or to execute problem-solving steps (e.g., Reif and Heller, 1982). Research has even been done on how experts' and novices' problem-solving strategies and abilities differ, including how they *select* equations when problem solving (Kuo, Hull, Gupta, and Elby, 2013). Examination of how individuals *use* these equations in the mathematical processing step has rarely if ever been studied in science education fields, let alone chemical education. Because of foundational role of mathematics in chemistry, it is of the utmost importance to understand *how* equations are used and understood by chemistry students.

Much more investigation into students' understanding and use of mathematics in physical science contexts is needed (Bain and Towns, 2016; Bain et al., 2014). Although, these studies do provide some insight, it is not entirely clear what aspects of mathematics are troublesome for students . It is not yet understood *how* students are using and reasoning about mathematical symbols and processes when solving the type of problems investigated in these studies. However, previous work does make it clear that students struggle to blend conceptual and mathematical reasoning. Student difficulty working at the interface between chemistry and mathematics is what underpins the motivation for this work.

Chemical kinetics

In the undergraduate chemistry curriculum copious amounts of quantitative problem solving occurs when learning topics that are traditionally considered analytical or physical chemistry topics, which appear both at the introductory and upper levels. Chemical kinetics is one of these contexts, which often appears in general, inorganic, physical, and biochemistry courses (and sometimes others as well). Though commonly taught in numerous courses, studies on students' understanding of chemical kinetics are relatively uncommon, especially when considering students at the university level (Bain and Towns, 2016; Justi, 2002). Much of the work in this area is presented in reviews by Justi (2002) and Bain and Towns (2016). These reviews reveal that studies are usually conducted with a sample of students at the secondary level, cataloguing alternative conceptions or studying targeted instruction (Bain and Towns, 2016; Justi, 2002). Foundational concepts, such as reaction rate, effects of different variables (e.g., temperature, concentration, or catalysts), and activation energy, are typically the focus of this body of work (Bain and Towns, 2016; Justi, 2002).

Cakmakci and colleagues noted in their studies that both secondary and university-level Turkish students typically focused on the macroscopic level, rather than the particulate (or theoretical) level, when describing or explaining phenomena (Çakmakci and Leach, 2005; Çakmakci et al., 2006; Çakmakci and Aydogdu, 2011). A difference between the two groups was that secondary students were more likely to use everyday experience or restatements of available information to justify their claims, whereas university-level students were more likely to engage in explanations based on a theoretical model or causal mechanism.

Little work has been done to study how students engage in chemical kinetics problem solving. A recent study by Becker et al. (2017) investigated how students reasoned about, constructed, and evaluated rate laws in a method of initial rates task. During this task, participants approached construction of the rate law in five different ways. Those at the top of the hierarchy still demonstrated some difficulty with the task. Further, they revealed difficulty understanding the nature and purpose of rate laws. This and other work has motivated this investigation into students' use and understanding of mathematics in chemical kinetics.

Theoretical perspectives

Two theoretical perspectives underpin this work: personal constructs and blended processing. The first, personal constructs, is a combination of personal and social constructivism (Kelly, 1955). It describes knowledge as being formed in the mind of the learner, but acknowledges the social aspect of learning, which often gives rise to similar knowledge constructions within groups. Blended processing, a framework from cognitive science, complements this perspective, as constructivism does not go into detail as to how different knowledge constructions interact, or "blend" (Coulson and Oakley, 2000; Fauconnier and Turner, 1998). This framework has been used in various contexts to explore human information integration (Bing and Redish, 2007; Coulson and Oakley, 2000; Fauconnier and Turner, 1998; Hu and Rebello, 2013). It provides a way to describe and understand individuals' knowledge constructions (or mental spaces) and their interactions (Bing and Redish, 2007; Hu and Rebello, 2013). Interactions involve two or more mental spaces selectively blending information from each space to make sense of cognitive input in an emergent fashion, also described as the blended space (Bing and Redish, 2007; Fauconnier and Turner, 1998; Hu and Rebello, 2013).

When designing this study, blended processing was chosen as a theoretical lens because of the interdisciplinary nature of chemical kinetics. Across undergraduate curricula, kinetics units often heavily utilize mathematical models, which serve as a language to communicate conceptual understanding and as a tool to describe chemical systems. In this work blended processing has functioned as a framework to characterize cognitive elements/processes involved in modeling and problem solving. The selection of this framework explicitly informed the design of this study, influencing many aspects such as the selection of participants, the design of the interview prompts, and data analysis. These are further discussed in the methods section below.

Methods

Participants

All participants were sampled from a large Midwestern university over the period of two semesters (fall and spring) (Table 1). Most of the participants in this study were recruited from a second-semester general chemistry course primarily for engineering majors, which met three times a week for instruction (50 minutes each) and once a week for lab (170 minutes). Additionally, upper-level students were recruited from a chemical reactions engineering course (a course for chemical engineering majors) and a physical chemistry for life sciences course (a course for biochemistry and various life science majors). The chemical reactions engineering course met four times a week for instruction (50 minutes each) and once a week for lab (170 minutes), whereas the physical chemistry for life sciences course met four times a week for instruction (50 minutes each) and did not have a laboratory component. Most introductory-level participants were first-year undergraduate students, and most of the upper-level participants were in their third or fourth year.

Table 1 Overview of participants interviewed by course and semester

Study population	Number of students interviewed	
	Fall 2015	Spring 2016
Pilot study (general chemistry II)	4	-
General chemistry II	17	19
Physical chemistry for life sciences	-	5
Chemical reactions engineering	-	3

Non-major science, technology, engineering, and mathematics (STEM) students were chosen as the study sample for two reasons. First, they are larger in population. Secondly, the ability to integrate different knowledge domains to solve a problem characterizes expert-like reasoning across STEM disciplines (Kuo, Hull, Gupta, and Elby, 2013). For this reason, we wanted to explore how students in a range of STEM disciplines solve problems. Participants were recruited prior to instruction on chemical kinetics and interviewed after completing the unit, as well as any accompanying assignments and exams.

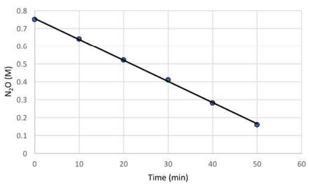
Interviews

The primary mode of data collection was individual, semi-structured interviews using a think-aloud protocol (Becker and Towns, 2012). Participant written work was recorded using a Livescribe™ smartpen capturing both audio and writing in real time (Linenberger and Bretz, 2012; Harle and Towns, 2013; Cruz-Ramírez de Arellano and Towns, 2014). The interview prompts were printed on Livescribe™ paper and probing questions for clarification and elaboration were verbally asked by the interviewer (King and Horrocks, 2010). Each participant was compensated with a $10 iTunes gift card. The study design and interview protocol were reviewed and approved by the Institutional Review Board.

The interview protocol design was inspired by Kuo et al. (2013), including two prompts that provided equations (*math prompts*) and two chemical kinetics prompts (*chemistry prompts)*. The full protocol including examples of probing questions is provided in the Appendix. In the math prompts that provided equations, participants were asked to explain either a second- or zero-order integrated rate law. The chemistry prompts were more "traditional" in nature, representative of a homework or exam problem from a chemical kinetics unit (Fig. 1). The problems selected for these interviews were designed because of their potential to help elicit conceptual understandings about chemical kinetics, as well as formal mathematical reasoning. Each problem could be solved using a conceptual understanding of kinetics and mathematical relationships; additionally, they could be solved using various kinetics equations and the provided experimental data.

A second-order reaction, $2\ C_4H_6(g) \rightarrow C_8H_{12}(g)$, was run first at an initial concentration of 1.24 M and then again at an initial concentration of 2.48 M. They were run under the same reaction conditions (e.g. same temperature). Data collected from these reactions are provided in the table. Is the rate constant for reaction 2 (1.24 M) greater than, less than, or equal to the rate constant for reaction 1 (2.48 M)?

Time (hrs)	$[C_4H_6]$ (M)	
	Rxn 1	Rxn 2
0	1.24	2.48
1	0.960	1.55
2	0.775	1.13
3	0.655	0.89
4	0.560	0.73
5	0.502	0.62
6	0.442	0.54
7	0.402	0.48
8	0.365	0.43
9	0.335	0.39
10	0.310	0.35



Below is a zero-order rate plot for the reaction $N_2O(g) \rightarrow N_2(g) + \frac{1}{2}O_2(g)$, where $[N_2O]_0 = 0.75$ M and $k = 0.012$ M/min. The reaction is conducted at 575 °C with a solid platinum wire, which acts as a catalyst. If you were to double the concentration of N_2O and run the reaction again, how would the half-life change? At the half-lives for each reaction run, how do the chemical systems compare?

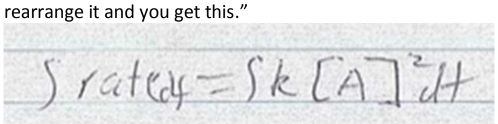
Fig. 1 Second- and zero-order chemistry prompts.

The order of interview prompts was alternated every other interview. For example, the first interview participant received a chemistry prompt (second-order chemical kinetics problem) and then a math prompt (second-order integrated rate law), whereas the second interview participant received the math prompt and then the chemistry prompt (the same pattern held for the third and fourth prompts involving zero order). We did this to determine if there were any priming effects in student responses when they saw mathematical equations before responding to the "chemistry" problem and vice versa.

Data Analysis

The interviews were transcribed verbatim. Images of student work were embedded into each transcript as well, using the real-time Livescribe™ data. The interview transcripts were then organized into "interpreted narratives," restructuring the data in a way that aided data analysis to investigate our research question (Page, 2014). To do so, we identified problem-solving "steps" that each student made when responding to each interview prompt. All data from each interview were organized into a table, chronologically, where each row in the table contained two columns: verbatim transcript data and a brief descriptor of the step (Table 2).

Table 2 Excerpt of Trip's interpreted narrative for problem requiring him to explain the second-order integrated rate law equation

Student's problem solving	Step
"Okay, so, this is the second order integrated rate law."	Recognizes equation
"And so, it starts with, you have your rate equation for a second order reaction. And then you, if you integrate both sides with respect to time. dt. Then you end up, and then you rearrange it and you get this." 	Recognizes origin of equation
"So, basically, the purpose of this is so you can have a function of concentration versus time. Instead of just concentration versus rate. That way it's easier to use in like the lab."	Highlights purpose of equation

Keeping in mind the framework of blended processing, an open-coding approach was used to analyze the interpreted narratives. This resulted in codes that described different ways of solving kinetics problems, many types of conceptual and mathematical understanding, and blended processing of varying complexity in several contexts (Fig. 2). Problem-solving codes described typical methods employed when working on the two chemistry interview prompts (e.g., provides appropriate equation or graphical approach). Student responses were also coded with respect to the content understanding they were expressing (e.g., conceptual understanding of catalyst or mathematical understanding of rate). Blended processing codes were used when students explicitly integrated chemistry and mathematics in their discussion (sometimes with accompanying handwritten representations). To represent the variance in this data, additional codes were developed to characterize blended processing in terms of the specific content category (context), movement from one mental space to another (directionality), and spectrum, in terms of the caliber of discussion (quality).

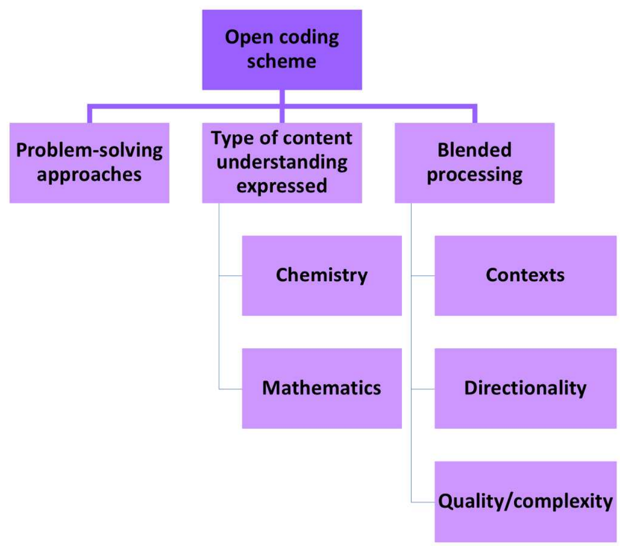


Fig. 2 The final open coding scheme had three broad categories of codes, which characterized approaches to problem solving, type of content understanding expressed (usually content related to chemistry and mathematics), and blended processing (instances when chemistry and mathematics were both used in an integrated fashion).

Frequently, codes were assigned to excerpts of data as they were organized into steps in the interpreted narrative, which meant that a single problem-solving step received one code. There were also instances where multiple codes were assigned to all the data in a single step or different codes were assigned to different parts of the data in a single step. Each of the interviews were coded by a team of two researchers, requiring 100% intercoder agreement (Campbell, Quincy, Osserman, and Pederson, 2013). That is, the two coders required 100% reconciliation of any coding discrepancies for all parts of each interview throughout the entire data analysis process. A constant comparison methodology was used to refine and modify the codes and their application throughout the data analysis (Strauss and Corbin, 1990).

Findings

Participants varied in the number and type of problem-solving routes used to address the prompts, as well as the range of students' ability to blend chemistry and mathematics. To communicate this variety, we utilize student quotes that exemplify observed responses. In the following sections, we describe the characterization of different blending facets (context, directionality, and quality) and discuss its role in problem solving across our sample (Fig. 2).

Common blending contexts

Molecularity and order. One topic students often discussed while blending was the idea of molecularity and its relationship to order. Consider Hank, a general chemistry student, who responded as follows when thinking about the second-order math prompt (Fig. 3).

Hank: *"If it's an elementary step, second order will mean that there will be two particles colliding together to form some stuff, and basically that's why it's second order. Second order just means that if you change the concentration of this reactant, this A reactant, say you change it by a factor of 2, the result on the rate will be, the amount of change introduced, squared. That's what second-order rate means."*

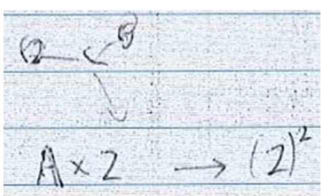


Fig. 3 Hank's written work depicted particle collision as well as the mathematical relationship between molecularity and the order exponent.

In this passage, Hank began by thinking about the molecular-level description of the reaction. He noted that two A molecules collide and connected this to the mathematical relationship, represented as a two in the exponent in the rate law. He went on to discuss how the rate would change if the concentration increased by a factor of two, which would be squared because of the second-order rate relationship. Hank thought about the chemistry behind the phenomenon and integrated this knowledge with a mathematical understanding of the process being modeled.

Catalysts. Students also frequently discussed catalysts while blending. For example, Steven, a general chemistry student, discussed catalysts in zero-order reactions:

Steven: *"If you add a solid or liquid catalyst, in general, that makes it a zero-order reaction due to the limited number of surface areas. … Which would make sense in a liquid or solid thing, because the surface area of those are much more defined than say, a gas. … It [the platinum wire catalyst] has basically a surface that has this many particles that can react, and that creates a constant rate of reaction. That doesn't hold up right at the beginning or right at the end [of the reaction], but for the majority of its life span, there's a middle that does hold up."*

In the passage above, Steven discussed the origin of concentration independence for zero-order reactions by explaining the role of the catalyst in the reaction. In his discussion, he related the particulate description of the catalyst, which has a finite surface area to facilitate reactions, to the mathematical implications for modeling rate, explaining the particulate-level implications for reaction rate and indicating the limits of the zero-order model as a constant-rate reaction at the beginning and end of an experiment.

Concentration. The most common topic that was discussed while blending was the idea of how the concentration of a reactant, [A], changed over time. In the passage below one of the general chemistry students discussed the zero-order integrated rate law (i.e., $[A] = -kt + [A]_0$), relating the graphical representation to the chemical phenomena it models (Fig. 4).

Serena: *"Negative kt, with negative just means negative slope, or a decreasing in concentration, so this [concentration of A] is definitely going down. The initial concentration of A, that number's going to get smaller and smaller. … A yields something else, B. … A goes to B. In order to produce B, more of A would have to be used up. So, while this gets used up, this gets produced."*

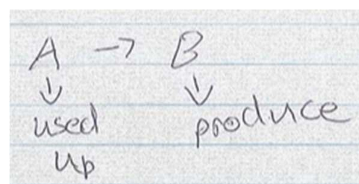


Fig. 4 Serena's written work further expanded on her discussion, supporting the connection made between the mathematical variable [A] and the chemical reaction.

Serena identified features from the equation, the negative *kt*, and considered how this reflected the nature of the change in concentration of the reactants, the variable [A]. She then tied this mathematical relationship to the behavior of reactant species during a reaction, blending ideas regarding aspects of the mathematical expression with chemical phenomena. More examples of this content theme are discussed later when we describe the observed differences in the quality of blending.

Directionality of blending

Within the identified instances of blending, there are indications that there is directionality associated with the student reasoning. In practice, blending often involves students starting in one mental space (e.g., chemistry) and then moving to or making connections with another mental space (e.g., mathematics). In some instances, this is less clear as students weave back-and-forth between chemistry and mathematics; in other cases, there seems to be a clear initial mental space in which a student anchors their reasoning. For example, in the passage that follows, Blair (enrolled in physical chemistry for life sciences) begins by thinking about chemistry, discussing enzymes and associated structural considerations (i.e., the number of active sites), and then moves into how this has mathematical implications for the rate.

Blair: *"An enzyme is a type of catalyst, and enzymes only have a specific number of active sites where the reactant or substrate could bind. So basically, your maximum rate is going to be when all of those active sites are occupied. Once you hit that point, you could have tons and tons, you could just keep throwing substrate at it, but it's not going to help you because you only have so many places on that enzyme where it could bind. That's a case that the rate is going to hit its constant when the catalyst is fully occupied. Any extra reactant beyond that is not going to change the rate, because the catalyst is doing the best it can. The catalyst does work to increase the rate of the reaction, but it can only do that until the point that it's fully saturated, fully occupied."*

In this example, Blair exhibited *chemistry to mathematics blending*, in which her chemistry understanding provided implications for mathematical quantities. She considered the physical system of an enzyme-substrate reaction and the implications it would have for a rate quantity (Fig. 5).

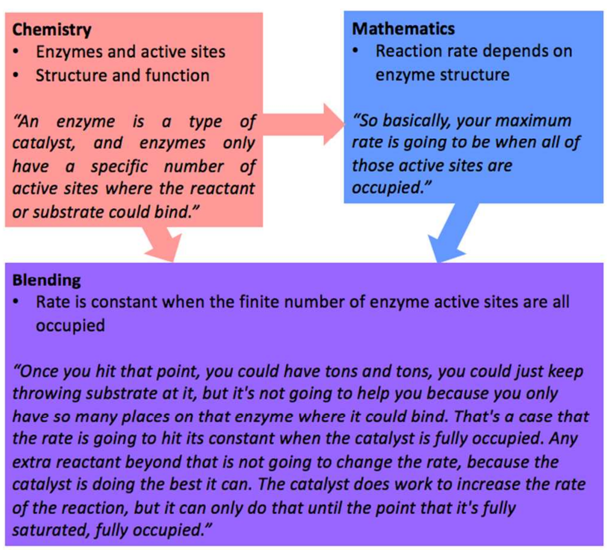


Fig. 5 Blair's discussion of enzyme catalysts and rate provides an example of blended processing that originated in the chemistry domain, considering the physical system of an enzyme-substrate reaction and its implications for rate.

However, among our participants, we more frequently observed *mathematics to chemistry blending,* where students attribute meaning to mathematical expressions. This can be seen in the passage below where Poppy, one of the chemical engineering students, thought about the implications of having a negative order. This passage comes after Poppy described the mathematical definition of order (exponent in the rate law) and its physical implications for elementary reaction mechanisms.

Interviewer: "*Have you encountered negative rate orders like that before, where they're a negative 1 or negative 2?"*

Poppy: *"Yeah. … We recently had a lab that we did. ... The negative 1 order ... That [tells you that] the presence of this molecule hinders the reaction. So, a lot of times it's associated with the concentration of water because water tends to hinder a lot of reactions for some reason. We always want to get water out of it."*

In this case Poppy began with the numerical value of the rate law exponents and considered what this could imply about a chemical reaction, providing a reasonable particulate-level description. She conjectured that the concentration of something raised to a negative exponent would slow the rate of a reaction; from her laboratory experience, she knew that that water sometimes hinders forward reaction progress, leading her to suggest that it could possibly appear in a rate law with a negative order value. With respect to instances of blended processing, this type of reasoning that is initially situated in mathematics occurred with a higher frequency than movement from chemistry to mathematics.

Although future studies need to be done to understand and characterize directionality of blending, our data reveal that students (unprompted) indicated they felt more comfortable using and reasoning with mathematics. In fact, this sentiment was shared so frequently that a code "*student prefers mathematics"* was created. This preference for mathematics is also supported when considering that across our dataset we observed students more often reasoning with mathematics than with chemistry. In the quote below, Damien, a general chemistry student, exemplified a common theme among the students: mathematical thinking and calculating afforded clearer answers when compared to conceptual reasoning.

Damien: "*Usually I go for the mathematical way. It gives the clearest results. … Usually mathematical results, result in the quickest way possible."*

This could be what led the participants to more frequently anchor their reasoning in mathematics and then subsequently attribute chemical meaning to the mathematics (rather than mathematizing chemistry understanding).

Quality of blending

Students also expressed variability in the quality of the blending exhibited—a blending spectrum. Furthermore, those that exhibited more instances of blending generally also exhibited a higher level of blending. For the purposes of this study we characterized student blended processing as either low or high. This can be seen when comparing two of the general chemistry students, Nate and Eric, who both discussed the previously mentioned content category of how [A] changes with time. Although the students discussed the same topic, the extent in which they made connections between chemistry and mathematics differed. For example, Nate stated:

Nate: "*The initial concentration does not change, but the final concentration would change, because if you're using a dissociation equation. ... Let's say A gives B plus C. Your A would be … diminishing over time, and B and C is being formed over time. … The A would change over time, and it would eventually lead to zero, which would convert completely into B and C under ideal conditions. … Your initial concentration of A*

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is what stays constant. Over time, the concentration of A keeps decreasing."

Here, Nate discussed the variable [A] in the second-order integrated rate law and attributed meaning, tying it to a possible chemical process and describing how it changes over the course of a reaction (which is similar to Serena's quote earlier). This contrasts with how Eric reasoned about the same variable in the context of the zero-order integrated rate law (Fig. 6).

Interviewer: "*In this equation … there is a negative kt. Why is that?"*

Eric: *"That's because A, as we're talking about, is a reactant, and this is a reaction that takes A and creates another product. Over time, A has to decrease, so the negative represents that k is just the value of how much A decreases over time or per unit of time as represented by t. It's like slope. … I'm drawing conclusions about slope because that's how I understand it. It's negative, because it's decreasing over time. … At zero, A is at this, and then per second, it decreases a set amount and that amount is k."*

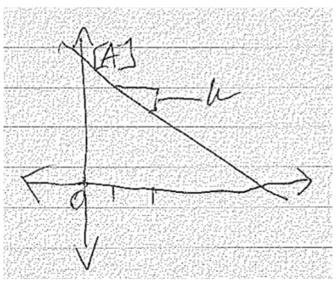

Fig. 6 Eric's written work further communicated his conceptions regarding the zero-order integrated rate law.

Comparable to Serena and Nate, Eric considered the equation and how the concentration, the [A] variable, changed over time, tying it to the nature of reactants in chemical reactions. However, in addition to making the initial claim regarding how the chemistry and mathematics relate, Eric built on this initial claim by considering other features of the zero-order integrated rate law, such as the negative sign, k, and t, and making connections to the graphical representation that he drew during this discussion (Fig. 6).

Comparison of blending among participant course level

Results suggest there may be a trend among participants in which blending is more likely to occur with the lower-level students than with the upper-level students. This was surprising because we assumed students that are further along in their education would be able to better integrate chemistry and mathematics in their problem solving, as it would reflect more expert-like thinking (Chi, Feltovich, and Glaser, 1981; Chi, Glaser, and Rees, 1982; Hull, Kuo, Gupta, and Elby, 2013; Kuo et al., 2013; Reif, 1983, 2008; Reif and Heller, 1982). However, initial analysis of course materials, such as the lecture notes and assigned textbooks, did not reveal any significant differences that could potentially explain trends in blending among participant course level, suggesting more work needs to be done to characterize students' ability to integrate chemistry and mathematics, focusing on how this changes over time across different academic levels.

Trends in problem solving

To identify if there was a relationship between blending ability and problem solving, we compared students that exhibited more instances of blending with students that did not engage in blended processing in their interview. For the purposes of analysis, we will refer to students that exhibited five or more instances of blending as *high-frequency blenders* (5 students meet this criteria) and students that did not blend during their interview as *non-blenders* (12 students meet this criteria). Cases in which students engaged in blending were characterized as distinct instances of blending when thematically distinct, that is, separated by topic discussed by the student. Generally, among the high-frequency blenders (4 general chemistry students and 1 physical chemistry student), students approached the problem by answering the prompts correctly with a conceptual justification, often following it up by supporting their claim with mathematical calculations (Table 3). In addition, this group of students tended to identify additional productive alternative problem-solving approaches (e.g., solving the problem using the integrated rate law and then discussing how they could have also solved the problem graphically) and were more likely to consider the implications of working with empirical data (e.g., using the data provided to solve for the rate constants and acknowledging that theoretically the k values should be equal, but they will vary slightly in practice when working with experimental data). This type of problem solving observed in high-frequency blenders is reminiscent of expert-like problem solving, where integration of conceptual and mathematical reasoning is a prominent characteristic (Hull et. al, 2013; Kuo et al., 2013; Reif, 1983).

In comparison, the non-blenders (8 general chemistry students, 2 physical chemistry students, and 2 chemical engineering students) exhibited more variation in problems solving, with students proportionally showing less ability or even attempts to approach the problems conceptually (Table 3). They often utilized multiple unproductive problem-solving routes and displayed a higher likelihood to reach incorrect conclusions based on their calculations. Furthermore, the non-blenders were more likely to suffer from "dead starts", in which the students do not provide an answer and indicate they are unable to solve the problem, and "dead ends", in which the students are unable to correctly answer the question after some initial progress (Bodner, 2015).

Table 3 Summary of problem-solving approaches among high-frequency blenders and non-blenders

	High-frequency blenders (n=5)	Non-blenders (n=12)
Typical problem-solving approaches	Students initially solved the problem conceptually, then supported their answer mathematically	More variation in problem-solving approaches with more "dead starts" and "dead ends", and less conceptual reasoning

Influence of prompt order on blending

The interview questions were grouped so that the students first did a chemistry and math prompt related to a second-order reaction and then they did a chemistry and math prompt related to a zero-order reaction (although the students were not explicitly told the relationship between the chemistry and math prompts). For our interviews, we alternated the order of the prompts to see if there were any priming effects: half of the participants had the math prompt before each chemistry prompt (*math-first students*) and half of the participants had the chemistry prompt before each math prompt (*chemistry-first students*). In terms of blending, the math-first students were more likely to engage in blending when compared with the chemistry-first students. In fact, all five high-frequency blenders were math-first participants. However, non-blenders were evenly distributed across the math-first and chemistry-first groups (six students in each group), suggesting that non-blenders were unable to blend regardless of prompting or any advantages that could be attributed to a priming effect.

Limitations

It is important to note that within our characterization of student blending, we are not stating that non-blenders are *unable* to engage in blending, but rather that the prompt did not elicit blending in this group of students; they may be able to blend in other contexts. Further, we assert that non-blenders could learn to blend in this context with support and scaffolding from instructors.

Considering the trends noted regarding the directionality of blending, it should be reiterated that this characterization was challenging because of the level of integration of chemistry and mathematics. Some student responses lacked clear framing from one mental space or another. Also, it could be suggested that the nature of the chemistry prompts influenced the fact that there were more instances of mathematics to chemistry blending. With the inclusion of data tables and graphs, the chemistry prompts may encourage students to think mathematically and potentially favor algorithmic approaches to solving the problems over a more conceptual approach. However, this is an artifact of how kinetics is commonly presented and assessed in chemistry courses and textbooks. The chemistry problems were chosen based on their similarity to problems students are exposed to in their courses, which could be related to the observed student preference for mathematical problem-solving approaches and the priming effects of the math-first prompt.

Finally, the sample size of upper-level participants limits the comparisons and claims that can be made when juxtaposed to the larger sample of general chemistry participants, requiring more research to be conducted with upper-level students. This exploratory work suggests possible differences in blending ability when considering frequency, quality, and directionality, though these must be further investigated and characterized.

Conclusions and implications

Why is blending important?

In work outside of physical chemistry, representations of phenomena are functionalized as *inscriptions*, which broadly encompass mathematical expressions such as equations and graphs; however, this can be a potential source of confusion for students, because as inscriptions become more powerful (in terms of the amount of information they communicate), they become more abstract and more disparate from the process it models (Becker and Towns, 2012; Lunsford, Melear, Rother, and Hickok, 2007). For this reason, when students see equations in chemical contexts, they may have difficulty attributing meaning, viewing it only in mathematical terms (Bain et al., 2014; Becker and Towns, 2012). The lack of clear surface-level connections between an equation and the system being modeled (e.g., a second-order integrated rate law and a reaction involving two molecules of buta-1,3-diene) makes it difficult for students to identify the underlying relationships and engage in the use of models.

National-level US organizations (such as the American Chemical Society and the National Research Council) acknowledge the importance of incorporating opportunities for students to engage in reasoning and activities that involve more than just content knowledge (Brandriet, Reed, and Holme, 2015; Cooper et al., 2015; Holme et al., 2015; National Research Council, 2012; Reed, Brandriet, and Holme, 2017; Wenzel, McCoy, and Landis, 2015). For example, the Next Generation Science Standards (NGSS) were developed, which are updated K-12 content standards framed around science practices that involve the integration of skills and knowledge to solve and approach problems (National Research Council, 2012). In addition to other skills, (e.g., engaging in argument from evidence) developing and using models was identified by the National Research Council (NRC) as foundational to the practice of science. Although the NGSS were written for K-12 education, modeling and other science practices are relevant for university-level education, particularly for chemistry, which relies heavily on the use of models of varying complexity (Brandriet et al., 2015; Cooper, 2013, Cooper et al., 2015; Reed et al., 2017; Taber, 2010).

The ability to blend across disciplines then becomes critical because it reflects the fine-grained reasoning that occurs as students model processes and combine chemical and mathematical descriptions. Thus, students that struggle to blend are likely going to face difficulties engaging in science practices. This goes beyond just the practice of developing and using models. All the NGSS science practices outlined by the NRC are deeply rooted in integration and blending of concepts at different levels, such as thinking about how empirical data and macroscopic observations translate to a particulate-level mechanism (the science practices of analyzing and interpreting data and constructing explanations) (National Research Council, 2012). Furthermore, the processes that are involved in blending mathematical and chemical descriptions could play a critical role in moving beyond thinking about a single, isolated phenomenon to promoting "systems thinking", which emphasizes the interconnectedness of multiple related systems (Mahaffy et al., 2017; Matlin, Mehta, Hopf, and Krief, 2016).

Chemical kinetics proved to be a productive context to explore students' ability to integrate chemistry and mathematics. The participants displayed a range in the quality and frequency of blending, along with variation in their problem-solving approaches. High-frequency blenders—students who were better able to integrate chemistry and mathematics—exhibited access to alternative productive problem-solving routes, allowing them to approach and think about the problems differently. These students displayed a deeper understanding of the chemistry phenomena being modeled, and we assert that blending is necessary for expert-like understanding across each of the core ideas in chemistry (structure and property relationships, electrostatic and bonding interactions, energy, stability and change), although it is not always taught (or deemed necessary to teach) at this level (Cooper, Posey, and Underwood, 2017).

How can instructors promote blending?

Promoting blending involves actively engaging students in tasks that involve modeling. Blended processing served as a way to characterize the cognitive processes involved in modeling as students reasoned about chemical kinetics. This characterization is critical so instructors can better aid students in working with models. In our analysis, we noted specific content categories that commonly served as a context for students to engage in blending, potentially providing good starting points to get students to think about integrating chemistry and mathematics. The prevalence of these topics suggests that these contexts are more accessible for the students. By making explicit connections between these mathematical inscriptions and the phenomena they model, we can help students view mathematical expressions as less abstract. We also suggest instructors provide examples for students that go beyond simple first-order and second-order reactions. By presenting reactions to students that are described using zero-order, negative-order, or fractional order kinetics, we can prompt students to think about the mechanism that is implied by the empirically derived rate law.

Our findings suggest that student ability to engage in blended processing may be supported by concurrent laboratory coursework that emphasizes the nature of mathematical expressions as deriving from descriptions of chemical phenomena. Although further work needs to be done to explore this, we noted that students enrolled in concurrent laboratory coursework more frequently discussed laboratory experience, experiments, and measurements. The physical chemistry students–which make up most of our upper-level sample–did not have a laboratory component to their course. While the small sample of upper-level participants limits our comparison, it is possible that this could contribute to the decrease of blending observed from the introductory- to upper-level. According to Driver et al. (1994), instruction should involve providing students an understanding of how "knowledge claims are generated and validated", and we posit that the laboratory setting provides an excellent opportunity for students to explore the theoretical and empirical basis of models, as well as their limitations, allowing students to gain a deeper understanding of the nature of scientific knowledge. Nevertheless, the extent in which laboratory courses influence a student's ability to make connections between chemistry concepts and mathematical expressions requires future investigation.

The data analysis and findings strongly suggest that students feel more comfortable utilizing mathematical reasoning, rather than chemistry. This could be a result of previous instruction, either due to increased exposure to mathematics over the course of a student's education, or perhaps it could be an artifact of a mathematics-centric presentation of chemistry in their courses. The fact the students are able to make connections by attributing meaning to inscriptions is encouraging and aligns with prior research (Becker and Towns, 2012); however, more support is needed to help students develop modeling ability in order to better reflect a "deep, transferable knowledge" that characterizes an expert's understanding of chemical phenomena (Cooper et al., 2015). Since students are displaying less movement from chemistry to mathematics, more guidance is needed to help students with the mathematization of chemical processes.

Equally important, since students focus their study efforts around what is assessed, both instruction and assessment need improvement (Cooper, 2015). Assessment needs to reflect a desire to teach and have students learn non-content goals such as blending, which move beyond rote memorization (Cooper, 2013; Reed and Holme, 2014). To promote blending, akin to that investigated and characterized herein, instructors must explicitly assess student ability to integrate chemistry and mathematics.

What future research on blending is needed?

The study described herein was exploratory in nature, adapting a framework from cognitive science to chemistry education research for the first time. The results suggest future avenues for further investigation. It would be useful to characterize trends among high-frequency blenders, such as their ability to engage in systems thinking or solve problems in novel contexts. It was also perhaps surprising to note that upper-level students were less likely to engage in blended processing, and it would be worth exploring how student ability to blend changes over time and what can be done to promote more frequent and higher-quality blending. Similarly, we are interested in the extent in which laboratory coursework influences a student's ability to engage in blended processing and modeling. Furthermore, more work is needed to consider the directionality of blending and potential reasons for observed patterns in directionality. Participants commented on their preference for thinking about and using mathematics instead of chemistry, which may be skewing student blending to be grounded in mathematical reasoning. We also assert the need for more research that investigates student mathematical reasoning. For example, characterizing mathematical reasoning in terms of the intuitive ideas students are attributing to mathematical expressions—similar to Becker and Towns' (2012) use of the Sherin's (2001) symbolic forms framework—may provide additional insight regarding how reasoning situated in mathematics influences students' problem-solving ability and understanding of chemistry.

Conflicts of interest

There are no conflicts to declare.

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Appendix

The characterization of cognitive processes involved in chemical kinetics using a blended processing framework

Kinsey Bain,[a] Jon-Marc G. Rodriguez,[a] Alena Moon,[b] and Marcy H. Towns[a]

[a]*Department of Chemistry, Purdue University, West Lafayette, Indiana, 47907, United States*

[b]*Department of Chemistry, University of Michigan, Ann Arbor, Michigan, 48109, United States*

Kinetics Study Interview Protocol (NSF DUE-1504371)

Thank you for agreeing to participate in this study on students' understanding of kinetics. During this interview you will be answering various questions. While you are thinking and working through each problem, I would like you to think aloud as you go. I will likely ask you follow-up or clarifying questions about the problem and what you are doing to try understand what you are doing and thinking as you work.

I am not here to determine if you are right or wrong. I simply want to know how you think about and work through these types of problems. This will be very helpful, as we want to help improve how we teach students about these concepts. Just a reminder, this will have no effect on your chemistry grade. This interview is confidential. I will keep your files and identity protected, and you will be given a pseudonym.

1. The second-order reaction, 2 $C_4H_6(g) \rightarrow C_8H_{12}(g)$, was run first at an initial concentration of 1.24 M and then again at an initial concentration of 2.48 M. They were run under the same reaction conditions (e.g., same temperature). Data collected from these reactions is provided in the table below. Is the rate constant for reaction 1 (1.24 M) greater than, less than, or equal to the rate constant for reaction 2 (2.48 M)?

Time (hrs)	**[C_4H_6] (M)**	
	Rxn 1	Rxn 2
0	1.24	2.48
1	0.960	1.55
2	0.775	1.13
3	0.655	0.89
4	0.560	0.73
5	0.502	0.62
6	0.442	0.54
7	0.402	0.48
8	0.365	0.43
9	0.335	0.39
10	0.310	0.35

Potential follow-up probing questions

How would you go about solving this problem?
What is this question asking? What information is given? How can you use it to reach an answer?
Do you need an equation to solve this problem? If yes, which one?
What is [A] in this problem?
How is [A] (or [C_4H_6]) changing? What does that mean is happening in the chemical reaction?
What is k? What type of information does this give you?
What is t?
Would your answer change if you were to compare this data to that of a different second-order reaction?
Do k's change from reaction to reaction? Why? How?
Is k always constant? (What could you change to make k a variable?)
Does your answer make sense to you?
(If they actually solved for rate constants and compared) Could you have answered this problem without doing calculations? How?
What does second-order mean? Mathematically? Chemically/physically?
What other reaction systems could be called second-order?
How does this mathematical model relate to the physical mechanism of the chemical reaction?
Could you have determined that this reaction was second-order mathematically? If so, how would you?

2. Here's an integrated rate law equation you may have seen in class/used above:

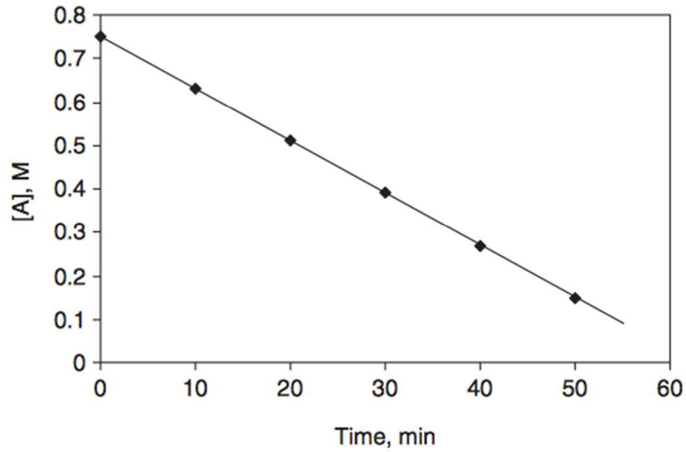
$$\frac{1}{[A]} = kt + \frac{1}{[A]_0}.$$

How would you explain this equation to a friend from class? How would you explain this on an exam?

Potential follow-up probing questions

What type of equation is this? (integrated rate law, linear function, etc)
What does [A] represent? What type of mathematical term (symbol) is it?
If they say [A] is a variable: What is chemically happening for [A] to change?
How are [A] and $[A]_0$ *different?*
What does t represent? What type of mathematical term (symbol) is it?
What is k? What type of mathematical term (symbol) is it?
What type of information does k give you? Can k tell you anything about the second-order reaction?
What are the units of k? Does that give you any insight to the chemistry that is happening? (physical information?)
Why are there only positive signs in this equation?
What order rate law is this?
How does this equation relate to a rate law? (Like those you would write in class?)
What is the purpose of each of the mathematical operations in this equation? (multiplication, division, addition)
What type of chemistry would correspond to this mathematical equation?
How was this equation derived? (From where did this equation come?)

3. Below is a zero-order rate plot for the reaction $N_2O(g) \rightarrow N_2(g) + ½O_2(g)$, where $[N_2O]_0 = 0.75$ M and $k = 0.012$ M/min. [A], M on the graph below represents $[N_2O]$ (M). The reaction is conducted at 575 ˚C with a solid platinum wire, which acts as a catalyst.



If you were to double the concentration of N_2O and run the reaction again, how would the half-life change? At the half-lives for each reaction run, how do the chemical systems compare?

Potential follow-up probing questions

How would you go about solving this problem?
What is this question asking? What information is given? How can you use it to reach an answer?
What is a half-life? What does that mean chemically? What does that mean mathematically? Or how would you determine a half-life mathematically?
How do you characterize chemical systems when they are at their half-life?
Do you need an equation to solve this problem? If yes, which one?
What is [A] in this problem?
How is [A] (or $[N_2O]$) changing? What does that mean is happening in the reaction?
What is a zero-order half-life dependent upon? Is this true for other orders? Why/why not?
Why would a half-life change for the same reaction run at different concentrations?
Does your answer make sense to you?
If you had not been told the reaction order, could you have determined the order from this plot?
What does zero-order mean? Mathematically? Chemically/physically?
What are typical causes for a reaction to be zero-order?
What role does the catalyst play with regards to the kinetics of the reaction? Mathematically? Chemically/physically? What would happen if you changed the amount of catalyst?
How does this mathematical model relate to the physical mechanism of the chemical reaction?
Would the order of reaction change without the presence of a catalyst? How? Why?
Does the catalyst interact with the reactants and products? If yes, how? How does the catalyst increase the reaction rate?

4. Here is another equation you've probably seen in class: $[A] = -kt + [A]_0$. How would you explain this equation to a friend from class? How would you explain this on an exam?

Potential follow-up probing questions

What type of equation is this? (integrated rate law, linear function, etc)
What does [A] represent? What type of mathematical term (symbol) is it?
If they say [A] is a variable: What is chemically happening for [A] to change?
How are [A] and $[A]_0$ different?
What does t represent? What type of mathematical term (symbol) is it?
What is k? What type of mathematical term (symbol) is it?
What type of information does k give you? Can k tell you anything about the zero-order reaction?
What are the units of k? Does that give you any insight to the chemistry that is happening? (physical information?)
What do the signs denote in this equation? (e.g. negative sign before the slope)
What order rate law is this?
How does this equation relate to a rate law? (Like those you would write in class?)
What is the purpose of each of the mathematical operations in this equation? (multiplication and addition/subtraction)
What type of chemistry would correspond to this mathematical equation?
How was this equation derived? (From where did this equation come?)
Compare to second-order equation? Why is there a different sign? Why is the concentration inverse in the second-order integrated rate law?