

Analyzing General Chemistry Texts' Treatment of Rates of Change Concepts in Reaction Kinetics Reveals Missing Conceptual Links

Sherry Seethaler,^{*,†} John Czworowski,[‡] and Lynda Wynn[§]

[†]Division of Physical Sciences, University of California, San Diego, La Jolla, California 92093, United States

[‡]Department of Chemistry, Grossmont College, El Cajon, California 92020, United States

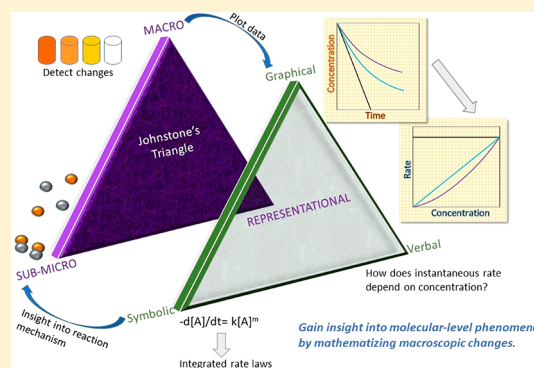
[§]Mathematics and Science Education Doctoral Program, University of California, San Diego, and San Diego State University, San Diego, California 92120, United States

Supporting Information

ABSTRACT: Change over time is a crosscutting theme in the sciences that is pivotal to reaction kinetics, an anchoring concept in undergraduate chemistry, and students' struggles with rates of change are well-documented. Informed by the education scholarship in chemistry, physics, and mathematics, a research team with members from complementary disciplinary backgrounds developed a rubric to examine how 10 general chemistry textbooks used by top producers of American-Chemical-Society-approved chemistry baccalaureates treat rates of change concepts in reaction kinetics. The rubric is focused on four categories of students' challenges that emerged from the literature review: (i) fluency with graphical representations, (ii) meaning of sign of rate of change, (iii) distinction between average and instantaneous rates of change, and (iv) connections between differential and integrated forms of the rate laws. The analysis reveals interesting patterns but also variability among the texts that, intriguingly, is not explained by the degree to which a text is calculus-based. An especially powerful aspect of the discipline-based education research lens is its ability to reveal missing conceptual links in the texts. For example, the analysis makes apparent specific gaps in the supports needed to help students move between representational forms (words, symbols, graphs) in the development of the differential form of the rate laws. The paper discusses the implications of the findings for chemistry instructors and chemical education research.

KEYWORDS: *First-Year Undergraduate/General, Chemical Education Research, Curriculum, Textbooks/Reference Books, Kinetics, Mathematics/Symbolic Mathematics*

FEATURE: Chemical Education Research



BACKGROUND

Discipline-based education research (DBER) provides considerable insight into the conceptual challenges of learning specific topics. Better supporting the translation of DBER findings into practice and conducting DBER at the intersection between disciplines are among the recommended goals for future research made by the National Research Council.¹ These two goals have motivated the study described here, which uses DBER as a lens to pose the following research question: How do general chemistry textbooks treat rates of change concepts in reaction kinetics? By “DBER as a lens” we are referring to a goal-oriented, two-stage process of first examining and synthesizing the literature on teaching and learning rates of change, and then crafting an analytical instrument with its constituent criteria directly emergent from the documented challenges faced by learners. Johnstone’s triangle, which connects three conceptual levels of chemistry (macro, submicro, representational), serves as a broad framework for

this study.^{2,3} The DBER lens developed here places particular scrutiny on Johnstone’s representational level.

The topic of this study was selected because scholarship in chemistry education, physics education, and mathematics education reveals widespread difficulties faced by students when learning about and applying rates of change concepts. The notion of change over time is fundamental to kinetics, which the American Chemical Society (ACS) Examinations Institute considers one of 10 anchoring concepts or “big ideas” in undergraduate chemistry.⁴ Textbooks were chosen as the object of study because they are required or recommended in most first-year chemistry courses, and because they provide a conceptual narrative that buttresses what students learn in class. In a recent study of over 1000 students in a dozen introductory

Received: March 30, 2017

Revised: October 3, 2017

science courses, more than three-quarters of students reported reading the textbook either often or sometimes.⁵

Reviews of the literature on teaching and learning chemical kinetics have compiled a plethora of student difficulties and misconceptions that commonly persist after instruction.^{6,7} The most recent of these reviews also highlights how mathematics education research on students' understanding of related rates can inform this area of chemistry education.⁷ Here we drew from the relevant literature in three disciplines (chemistry education, physics education, mathematics education) to create a list of students' rates of change challenges, which we then considered in the context of introductory reaction kinetics. At this intersection emerged four broad areas of student difficulties: (i) drawing and interpreting graphs to understand change over time, (ii) interpreting the sign in a rate of change, (iii) distinguishing average and instantaneous rates of change, and (iv) basic conceptual meaning behind derivatives and integrals.

Graphical Representations

Undergraduate chemistry students have difficulty constructing and interpreting graphs, and may experience anxiety with chemistry problems that involve graphs.^{8,9} Graphing problems that are purely mathematical prove less difficult than problems involving the same mathematical content in a physical context that introduces the need for translation of the context into mathematical language.^{10–12} Students also face challenges when integrating process skills such as graphing and comprehending chemical events in a microworld.¹³ Because it appears challenging for students to generalize the rate concept as change over time, their interpretation of graphs is dependent on the domain context as well as problem format.^{14–16}

When asked to sketch graphs of reaction rate versus time, a significant number of chemistry teachers produced graphs with unrealistic slopes, such as slope increasing exponentially without decreasing.¹⁷ High school students and undergraduate students also had difficulty sketching accurate reaction rate versus time graphs, even when they were able to provide accurate verbal descriptions of how the rate of a chemical reaction changes over time.¹⁸ Because curved graphs involve changes in both height and slope, students find them more difficult to interpret.¹⁹ Giving students the opportunity to predict the shapes of graphs and then compare the actual graphs with their predictions may be especially suited to promoting conceptual change.^{20,21}

Translating back and forth between different types of graphs also presents challenges.¹⁹ Students commonly expect graphs to remain the same after the variables on the axes are changed.^{15,20} They fail to distinguish between rate versus time, rate versus concentration, and concentration versus time graphs.¹⁸ Following traditional instruction in reaction kinetics, the vast majority of first-year undergraduate students incorrectly predicted that the reaction rate versus time graph would be the same as the concentration versus time graph.¹⁶ The opportunity to explore the relationships between graphs can help students develop a more intuitive feel for doing so.²²

Sign of Rate of Change

Studies have documented undergraduate students' difficulties with negative rates of change in various contexts, including kinematics (the meaning of negative velocity and negative acceleration), light intensity over distance from a point source, and discharge of a capacitor in a simple circuit.^{19,23} For example, when determining whether something is slowing

down or speeding up, students may base their responses on the sign associated with the slope of the position versus time graph, rather than the change in magnitude of the slope.¹⁹ They struggle to attend to the magnitude or absolute value and the sign of the rate of change simultaneously, and find it especially confusing when rates are negative but increasing in magnitude.²³ When solving equations or interpreting graphs, students commonly confuse the sign of the slope with the sign of the y -coordinate, or carelessly drop the negative sign.^{15,24} These findings have implications for curricular treatment of the negative sign associated with consumption of reactants.

Distinction between Average and Instantaneous Rates of Change

Over the course of a chemical reaction, rate may remain constant (zeroth-order), change linearly (first-order), or change nonlinearly (second- and other orders); the distinction between average and instantaneous rates of change is thus central to understanding relationships in reaction kinetics. Unfortunately, students fail to distinguish initial rate, instantaneous rate, and average rate over a time interval.¹⁸ They have difficulty saying how the rate of reaction changes over time, and confound constant and variable rates of change.^{7,25} A student who is able to apply a procedure to calculate average rate of change may not be able to explain the meaning of the average rate of change.²⁶

Representationally, average and instantaneous rates of change can be distinguished in words, graphically (slope of the secant versus slope of the tangent), and in symbols (Δ versus d), and moving between these representations presents a suite of difficulties for students. Many undergraduate students struggle with matching a text description with a graphical representation.¹⁹ They have a poor understanding of the symbol Δ .¹⁵ They may not understand that the average rate equals the instantaneous rate on a linear graph.²⁷ They often compute the slope at a point by simply dividing the y -value by the x -value.^{19,20} They may not view the tangent as the limit of the set of secants.²⁸ This research demonstrates that curricular support is needed to help undergraduate students develop fluency with moving between these rates of change representations, which are all relevant to understanding average and instantaneous rates of concentration change in introductory reaction kinetics.

Meaning of and Connections between Derivative and Integral

Students who have completed an introductory calculus sequence still commonly treat variables as symbols to be manipulated, rather than quantities to be related.²⁹ The differences between high school and undergraduate are not significant for the first course in differential and integral calculus, although undergraduates may have further lost touch with earlier mathematical knowledge and skills, such as graphing, and ceased to think in terms of rate of change.^{24,30} Even when students do have an understanding of rate when working with one kind of representation or context, this understanding does not necessarily transfer to other situations.³¹

A core principle in calculus (the fundamental theorem of calculus) is that the accumulation of a quantity (determined by integration) and the rate of change in the accumulation of the quantity (determined by differentiation) are interrelated.³² This principle, of course, underlies the connection between the rate laws in their differential form and in their integral form. Ideally,

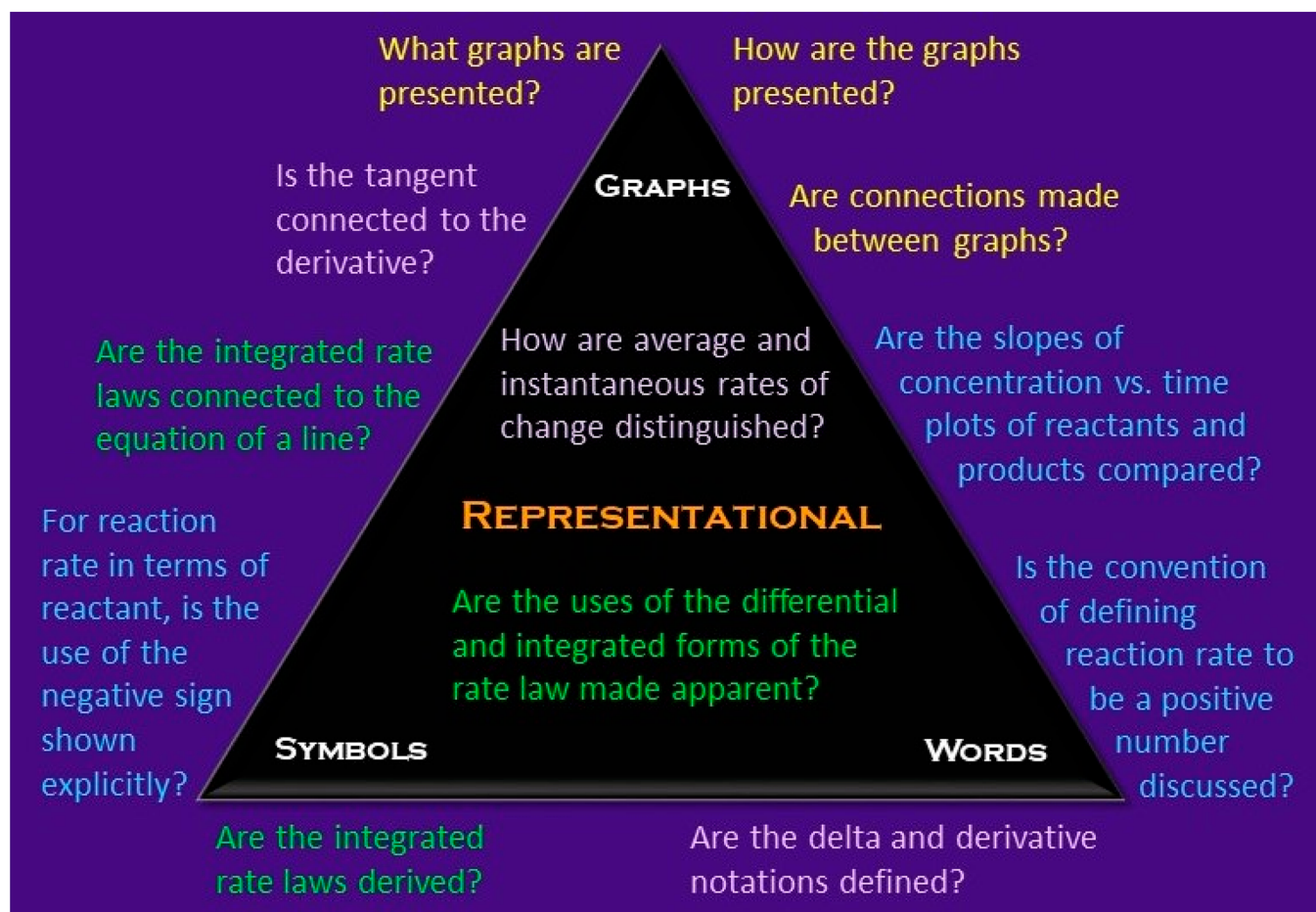


Figure 1. Supporting students to navigate the representational level of Johnstone's triangle. Color indicates the category of student difficulty: graphical representations (yellow), sign of rate of change (blue), distinction between average and instantaneous rates of change (lavender), and meaning of and connections between derivative and integral (green). To roughly indicate which representational level(s) are relevant for a particular question, the questions are positioned near a vertex, on a side between vertices, or between all three vertices (within the triangle).

students who have studied calculus would have internalized this basic idea and its implications, but this does not appear to be the case. Students frequently confound "amount" and "rate of change of amount" in general, and in particular, confound the rate of consumption of reactants with the amount of reactants during a reaction.^{14,25} They cannot correctly explain the meaning of terms in a differential equation, and mix up the function and its derivative.²⁵ Relevant to integration, students do not know what the area under the graph means.¹⁵ Finally, students who understand the terms in $y = mx + b$ and recognize it as the equation of a straight line cannot necessarily see the same (y -intercept, slope) relationships when other variables are involved.¹⁴ Although not strictly a calculus issue, fluency with the equation of a line is relevant to working with the integrated rate laws. These gaps in students' understanding of the connections between, and conceptual meaning of, the derivative and integral may not interfere with students' ability to plug and chug their way through simple kinetics problems, but such a piecemeal understanding will make it difficult for students to understand why they are doing what they are doing and apply their knowledge in new contexts. Highlighting this issue, a study that examined students' ability to use calculus concepts in a physical chemistry context presented a case of a student who had taken six semesters of undergraduate mathematics and could interpret the derivative in a

mathematics context, but could not use it to express change in a thermodynamics context.³³

The preceding discussion of the categories of students' difficulties with rates of change concepts underlying reaction kinetics underscores the particular challenges posed by the representational level of Johnstone's triangle.^{2,3} In reaction kinetics, various representations of macroscopic changes (i.e., of concentration) are created and manipulated to gain insight into molecular level phenomena (i.e., reaction mechanism). The representational level can be thought of as a "triangle within a triangle", involving navigation between graphical, verbal, and symbolic representations. For each category of student difficulty discussed above, Figure 1 shows where questions about how texts address that area of difficulty fit within the representational level.

Given the extensive literature on students' challenges with these conceptual underpinnings of reaction kinetics, it is valuable to examine to what extent textbooks make the relevant connections explicit. Various studies have examined the content of chemistry textbooks: documenting the analogies used to explain abstract chemical concepts, creating a taxonomy of end-of-chapter problems, and examining linguistic characteristics and depth of cohesion of the narrative.^{34–36} One paper has previously pointed out the failure of chemistry texts to clarify that the rate and rate constant are ambiguous in the absence of an explicit statement of the balanced reaction equation to which

they apply.³⁷ The analysis presented here contributes to the research on textbooks by providing insight into the collective strengths and weaknesses of textbooks in handling rates of change concepts in reaction kinetics.

METHODS

Texts

The texts analyzed were the general chemistry textbooks assigned by the top producers of ACS-approved chemistry baccalaureates.³⁸ The textbooks used by the top 10 ACS-degree producers were all included, except one (Zumdahl), which did not have a chapter on reaction kinetics.³⁹ Books by unique authors used by the next five producers were also included. To avoid real or perceived bias, one book by Tro (*Chemistry: Structure and Properties*) was not scored because another text by Tro was already included in the top 10. Because three textbooks (OpenStax, Oxtoby, and Tro's *Chemistry: A Molecular Approach*) were each represented twice on the list of top 15 ACS-degree producers, the score summary includes a total of 10 textbooks (referred to hereafter as Atkins, Brown, Chang, McMurry, McQuarrie, Oxtoby, Silberberg, Tro, OpenStax, UT Austin).^{40–49} The latter is an online text designed for a specific course, and because its videos were core (not supplemental) materials, their content was included in the analysis.

Raters

Three raters provided insights from different disciplinary perspectives. One rater was trained in chemistry (undergraduate and doctorate) and has taught introductory chemistry extensively at the undergraduate and community college level. One rater was trained in chemistry (undergraduate) and science education (doctorate). One rater was trained in mathematics (undergraduate and master's) and mathematics education (current Ph.D. student).

Scoring

The team developed the rubric based on the literature, and then iteratively refined it. The three raters independently scored all the texts. Initial interrater reliability was 85% (i.e., initial three-way agreement on 205 of 240 codes across the texts). Discussion of the relevant narrative passages or figures resolved the initial disagreements. Final interrater agreement was 100%.

Rubric and Research Questions

The rubric (see Table 1) was developed to investigate texts' treatment of rates of change concepts from the beginning of the kinetics chapter(s), through rate expressions and the differential form of the rate law, up to and including the presentation of the integrated rate laws. Depending on the organization of the text, this was an entire chapter, or the portion of the chapter before the sections on reaction mechanisms and catalysis. The rubric comprised the four categories of students' challenges with rates of change concepts relevant to reaction kinetics.

What Graphical Representations Are Used and in What Ways? The finding that students have difficulty predicting the shapes of rates of change graphs raises the question of whether texts give students the opportunity to do so. It is feasible for a textbook to include reflection prompts in the flow of the narrative or in the margins, prior to the introduction of fundamental graphs. The rubric asks about the presence of such prompts.

Table 1. Code Summary for All Textbooks Analyzed^a

Rubric Categories and Questions Investigating the Treatment of Rates of Change Concepts in Selected Textbooks ^a	Present?	
	Yes	No
Use of Graphical Representations to Introduce the Topic		
1 Are students encouraged to predict the shapes of any reaction kinetics graphs?	1	9
2a Does the text juxtapose graphs/other visuals side by side to explain concepts or draw attention to distinguishing features? ^b	10	0
2b Does the text use the technique of plotting multiple lines or curves on the same graph for explanatory purposes? ^c	8	2
3a Does the text present the relevant reaction kinetics graphs:		
(i) Concentration (or pressure) versus time?	10	0
(ii) Rate versus time?	2	8
(iii) Rate versus concentration?	5	5
(iv) Natural logarithm of concentration versus time?	10	0
(v) Inverse of concentration versus time?	10	0
3b Are other graph types presented?	4	6
Sign within the Rate of Reaction Definition		
1a Is it made clear that		
(i) Rate of concentration change of a reactant is negative?	10	0
(ii) A negative sign is added to make a positive quantity?	9	1
(iii) This sign change is a convention to express the rate equivalently for all substances involved?	6	4
1b Is it implied (incorrectly) that a negative rate of change does not make sense?	0	10
Distinction between Average, Instantaneous, and Initial Rates of Change		
1a Are at least two of these distinguished in		
(i) Words?	9	1
(ii) Symbols?	6	4
(iii) Graphs?	7	3
1b Are the Δ and derivative notations defined?	3	7
2a For the concentration versus time graph, is the limitation of the rise/run slope calculation (secant) explained with reference to the tangent?	7	3
2b Is the connection between the derivative and tangent made explicit?	3	7
Introduction of the Integrated Rate Laws		
1 Does the text explain what one can learn from the differential form of the rate law compared to what one can learn from the integrated form and why (i.e., emphasizing the variable of time)?	9	1
2 Does the text show or explain how the integrated rate laws are derived?	5	5
3 Is the connection to $y = mx + b$ made explicit for each integrated rate law?	10	0

^aThe codes for each individual textbook of the 10 examined are available in the Supporting Information. ^bMedian number of juxtapositions per text = 3; mean = 3.2; range = 1–6. ^cMedian number of composite plots per text = 2; mean = 2.2; range = 0–5.

For students to move between reaction kinetics graphs (e.g., concentration versus time, rate versus concentration, rate versus time) and infer the shape of one from another, students must, at minimum, be exposed to these different graphs. Thus, the coding scheme documents what types of graphs are present at least once in the text. Thoughtful juxtaposition of different types of reaction kinetics graphs, as well as graphs alongside other representations, is needed to support students' fluency of movement between them. The coding scheme asks what graphical representations texts juxtapose, either as separate figures or via the inclusion of multiple data plots on the same graph.

Table 2. Compilation of Juxtaposed Graphs and Visuals from Selected Textbooks and Their Purpose

Examples of Juxtaposed Graphs and Visual Elements	Pedagogical Purpose of the Visual Elements
Graphs of reactant concentration, natural logarithm of concentration, and inverse of concentration versus time (all).	Demonstrate how to determine reaction order from characteristic integrated rate law plots.
Graph of reactant concentration (or $[A]/[A]_0$) versus time with grid/molecular depictions showing concentrations at successive half-lives (Atkins, Chang, McMurry, Silberberg, Tro).	Connect to the molecular level to show how the concentration of a reactant decreases from one half-life to the next in a first-order reaction.
Graph of reactant and product concentration versus time with molecular depictions showing their concentrations at different times (Chang).	Similar to the half-life graphs (see above) but both reactants and products are shown and time points do not correspond to half-lives.
Graphs of reactant concentration versus time and rate versus concentration (Silberberg and Tro).	Compare how the reactant concentration varies over time and how rate varies with concentration for zeroth-, first-, and second-order reactions.
Graphs of concentration versus time and rate versus time for zeroth-order reaction (Atkins).	Show that, for a zeroth-order reaction, reactant concentration falls at a constant rate and reaction rate is constant (until reactant is completely consumed).
Graphs of rate versus reactant concentration and rate versus reactant concentration squared (Atkins).	Illustrate that a rate can be directly proportional to the square of a reactant's concentration rather than concentration to the first power.
Plot of absorption of bromine versus wavelength for four concentrations with photo of corresponding bromine solutions (Chang).	Connect the visible color change to shape of the absorption spectrum.
Concentration versus time graphs for reactants and products, comparing two different reactions side by side (Silberberg).	Introduce the rate expression by showing that the relative rates of reactants and products depend on their stoichiometric coefficients.

How Is the Sign of Rate of Change Treated? The positive or negative sign associated with a rate of change carries meaning. In kinematics, the sign provides information about direction of motion; in kinetics, the sign provides information about whether a chemical species is consumed or produced. Because it is clear from the literature that interpreting the sign of a rate of change is troublesome for students, it is useful to examine how textbooks deal with the sign in reaction rate. The rubric asks if the texts explain the meaning of the sign, and if they make clear that the definition of reaction rate as a positive quantity is a convention.

How Are Average and Instantaneous Rate Distinguished? Because students have difficulty with the distinction between rate of change over time and rate of change at one point in time, and because this distinction is fundamental in reaction kinetics, it is important that texts elucidate the distinction between average and instantaneous rate of change, ideally in words, symbols, and graphs. Recognizing initial rate of change as a subcategory of instantaneous rate of change is pertinent to the method of initial rates. Therefore, the coding examined texts' distinction of these three rates of change (average, instantaneous, initial) in the three modes of presentation (words, symbols, graphs).

What Scaffolds Are Provided To Help Students Understand and Connect the Differential and Integrated Forms of the Rate Laws? Even if students have taken an introductory calculus sequence before they study reaction kinetics, mathematics education scholarship demonstrates that they are unlikely to have more than a rudimentary understanding of the meaning of a differential equation or integral. Therefore, in introducing reaction kinetics, texts must elucidate critical connections, such as the connection between the slope of the tangent and the instantaneous rate, and the way integrating the differential form of the rate law brings in the variable of time. The rubric examines texts for these connections, which can be made conceptually whether or not the text is calculus-based.

RESULTS AND DISCUSSION

Graphical Representations

In general, the texts do not provide prompts to encourage students to predict the shapes of reaction kinetics graphs, although one text (Brown) partly did this in "Go Figure" and

"Give It Some Thought" prompts, for example, showing molecular depictions of reactants and products at three time points and asking students to estimate the concentration at an intermediary time.

The study revealed considerable variation in terms of what graphs texts use to build up to and introduce the rate laws. On one hand, all 10 texts present graphs of the following: concentration (or pressure) versus time, natural logarithm of concentration versus time, and inverse of concentration versus time. On the other hand, only two texts (Atkins and McQuarrie) present graphs of rate versus time, and only half the texts present graphs of rate versus concentration. The texts include a few other graph types: rate versus square of concentration (Atkins), a femtosecond spectrum illustrating decomposition of a halide (Atkins), plots of absorbance versus wavelength for solutions at different concentrations (Brown, Chang), and a bar graph showing the influence of the rate law exponent on rate (McMurry).

In terms of encouraging students to move between representations, the extent to which texts juxtapose two graphs, or a graph and another visual, also varies. The median number of juxtapositions per text is 3 (range 1–6). The most common use of juxtaposition is of the characteristic integrated rate law plots, with all the texts juxtaposing at least two of the three. The second most common juxtaposition, present in five texts, is a plot of concentration versus time with depictions of containers filled with spheres, dots, or squares that represent reactant concentration initially and at successive half-lives. In one text, a similar graph/dot juxtaposition shows the number of reactant and product molecules every 10 s.

Notably, in introducing the differential form of the rate laws, only three texts juxtapose graphs to compare relationships between concentration and time, and rate and time or concentration. One text juxtaposes a graph of concentration versus time with a graph of rate versus time. Two texts juxtapose a graph of concentration versus time with a graph of rate versus concentration. Table 2 is a compilation of juxtaposition types found in the 10 texts.

As is the case with juxtapositions, the extent to which texts use the technique of comparing multiple data sets on the same graph is highly variable. Median number of multiplot graphs per text is 2 (range 0–5). Most common are graphs of concentration versus time showing both reactants and products (Chang, McMurry, McQuarrie, Silberberg, Tro, OpenStax);

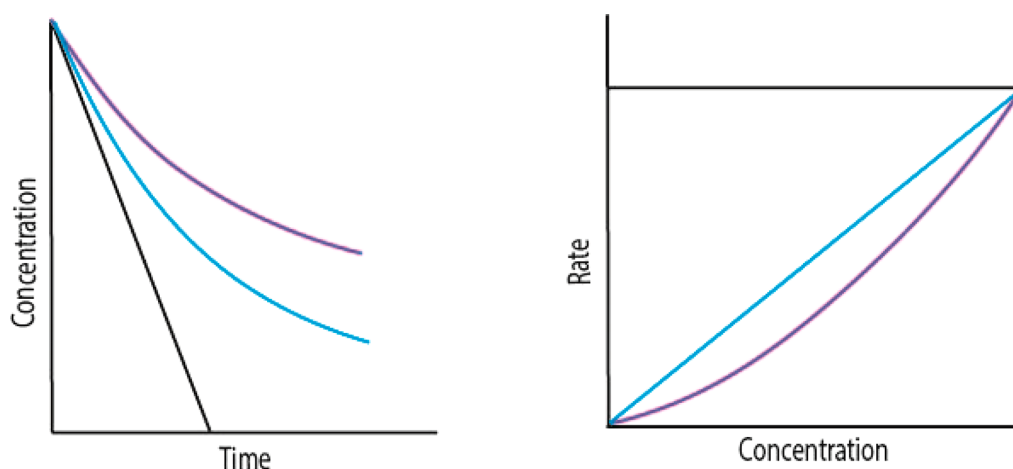


Figure 2. Juxtaposition of graphs of concentration versus time and rate versus concentration for a zeroth- (black), first- (blue), and second- (purple) order reaction.

another text shows reactants and products on a femtosecond spectrum (Atkins). Four texts compare plots for different reaction orders on the same axes: reactant concentration versus time for a zeroth- and first-order reaction (Brown, OpenStax); concentration versus time for a first- and second-order reaction (Atkins); concentration versus time for a zeroth-, first-, and second-order reaction (Silberberg and Tro); and rate versus concentration for a zeroth-, first-, and second-order reaction (Silberberg and Tro). Figure 2 juxtaposes these two latter multiplot graphs, as presented in Silberberg and Tro. Only one other multiplot figure appears in more than one text: absorbance versus wavelength for different concentrations (Brown, Chang). One text (Atkins) presents three multiplot graphs not used by other texts: concentration versus time for various initial reactant concentrations, concentration versus time for several rate constants, and ratio of current to initial reactant concentration versus time to show dependence of half-life of a first-order reaction on the rate constant.

Sign of Rate of Change

When introducing the rate expression, all the texts point out that the rate of concentration change of a reactant is negative. All but one (Oxtoby) indicate that a negative sign is added to make the rate of reaction a positive quantity. Six of the texts (Atkins, Brown, McMurry, Silberberg, Tro, OpenStax) point out that this is a convention (or because rate of reaction is defined as a positive quantity). None of the 10 texts scored here stated or suggested that the negative sign does not make sense; however, a statement to this effect was noted in another online text:⁵⁰

*Since negative rates do not make much sense, rates expressed in terms of a reactant concentration are **always** preceded by a minus sign to make the rate come out positive.*

Average and Instantaneous Rate

Words. All the texts except one (UT Austin) distinguish average, instantaneous, and initial rates of change using words. The texts, except three (Tro, UT Austin, OpenStax), also explain the difference between the tangent and the secant in terms of the time interval being considered.

Graphs. Three texts (Atkins, McMurry, Silberberg) use graphs to distinguish average, instantaneous, and initial rates. Two texts (McQuarrie, Oxtoby) distinguish average and instantaneous (but not initial) rates graphically, and two texts (Brown, OpenStax) distinguish instantaneous and initial (but

not average) rates graphically. The remaining three texts do not use graphs to distinguish the different kinds of rates.

Symbols. All the texts use the delta (Δ) notation. Four texts (McMurry, McQuarrie, Silberberg, OpenStax) do not use the derivative (d) notation; however, of the texts that use the Δ and d notation, only three (Atkins, Brown, Oxtoby) defined both notations. The remaining three texts (Chang, Tro, UT Austin) use both notations without defining them.

Differential and Integrated Forms

In terms of the use of calculus in introducing the integrated rate laws, the texts examined fell into three categories: narrative presenting integrated rate laws without deriving them (Brown, McMurry, McQuarrie, Silberberg, OpenStax), integration shown as an aside in margin (Chang, Tro), and integration central (Atkins, Oxtoby, UT Austin). Presence or absence of calculus steps, however, does not predict a text's treatment of the relationship between the tangent and the derivative. Only three texts, two of which are calculus-based (Atkins and Oxtoby) and one of which presents no calculus (Brown), explicitly state the connection between the tangent and the derivative. Another text (OpenStax) mentions that calculus is used to evaluate the slope of tangent lines. The connection between the tangent and the derivative, and the difficulty of finding the tangent by hand, can help establish the need for the integrated rate laws. As stated in Atkins (p 592)

Because it is difficult to draw a tangent accurately by eye, it is better to use a computer to analyze graphs of concentration against time. A superior method—which is described in Topic 7B [Integrated Rate Laws]—is to report rates using a procedure that, although based on these definitions, avoids the use of tangents altogether.

For the most part, the texts fail to provide this chain of logic, and two texts (Brown, Chang) calculate the slope of the tangent using the rise over run calculation (the same as they use for calculating the slope of the secant), without mentioning that doing so by eye is error-prone. Overall, the texts did a better job of explaining what one can learn from the integrated rate laws, with reference to the variable of time, and reminding students about the equation/graph of a straight line in connection to the integrated rate laws.

Two additional aspects of the texts' mathematics coverage deserve mention. The first concerns the meaning of symbols. The coder with the mathematics/mathematics education

background noted that students may not have encountered the proportionality (\propto) symbol or the double inequality (\gg) symbol in lower division mathematics classes, and furthermore, these symbols may have different meanings in other contexts. Along with the observation that some texts use the derivative notation without defining it, this underscores the importance of defining symbols.

The second aspect of the texts' mathematics coverage concerns mathematical integrity. Most of the texts that presented the integrated rate laws use single variables in multiple ways within an individual definite integral. This stood out to the coder from the mathematics/mathematics education background (but not to the coders from chemistry backgrounds, until it was brought to their attention). To illustrate, consider $\int_0^c \frac{1}{c^2} dc = -2k \int_0^t dt$. Note that c is used as an upper limit of integration \int_0^c , a variable in the integrand $\frac{1}{c^2}$, and the variable of integration dc (similarly for the t on the right side of the equation). Mathematicians distinguish between the limits of integration and the variables of integration. For example, they may write the above equation as $\int_0^{c_1} \frac{1}{c^2} dc = -2k \int_0^{t_1} dt$, or simply use different variables for the limits of integration. To do otherwise muddies the distinction between values and variables, another area the mathematics education literature points to as a source of difficulty for students.^{51,52}

■ IMPLICATIONS

The decisions made by curriculum designers may be conscious or unconscious. Writing a textbook involves conscious trade-offs between pedagogy and practicality due to publishers' limitations on length, layout, number of figures, and available color palette; moreover, in omitting or including calculus derivations, textbook authors are making conscious choices to appeal to specific audiences. Similarly, the author of every textbook in this study recognized the need to explicitly connect $y = mx + b$ with the integrated rate laws. Texts also had explanations about logarithms and exponents; one even included a figure to help students visualize how changing the exponent in the differential form of the rate law affects the reaction rate.

Yet, the most powerful aspect of the DBER lens is not in assessing these conscious choices to help students negotiate the representational level, but in revealing unconscious decisions. By definition, the DBER lens places the learner's understanding of a topic at the center of the analysis. Viewed from the learner's perspective, "adding in" a negative sign to make the rate of disappearance of reactant a positive quantity is puzzling and at odds with students' prior mathematics experience. It is unlikely to be a conscious pedagogical choice that some texts lacked a clear statement that this practice is a convention to express reaction rate equivalently for reactants and products.

Likewise, conceptual connections necessary to help students move from the differential form of the rate law to the integrated rate laws are often unconsciously glossed over, including the following: the graphical distinction between average and instantaneous rates of change, visual depictions of how the reaction rate changes over time or concentration, the limitation of the rise over run slope calculation, and the relationship between the derivative and the tangent. These choices are not attributable to the calculus level of the text. For example, the

non-calculus-based OpenStax textbook explains that calculus is needed to determine the slope of the tangent; in contrast are the texts that unproblematically calculate the slope of the tangent using rise over run. The DBER lens thus highlights where reaction kinetics instructional materials neglect the learner-centered perspective, which may inadvertently encourage rote learning and seed the prevalent postinstruction misconceptions documented in the literature.

These findings also provide actionable insights for chemistry instructors and chemistry education researchers.

Chemistry Instructors

Many factors, including cost, influence textbook choice, and individual instructors may not be free to choose the course textbook when the decision is made at the departmental level. This study provides criteria to help instructors "troubleshoot" their textbooks, and design lessons and select supplemental course materials to complement the text. DBER recommends that students be given the opportunity to predict the shapes of graphs and compare their predicted graphs with actual data, but textbooks do not provide this opportunity. Instructors could address this through small group work or clicker questions with whole class discussion, by having students sketch graphs or select from multiple-choice options and explain their choice. For example:

- Which of these graphs do you think best depicts how the concentration of the reactant will decrease over time: linear decrease, sharply decreasing slope that levels off, or level slope that subsequently drops off more rapidly?
- What do each of these graph shapes mean about the progress of the reaction? (See also ref 21.)

Similarly, instruction can delve into how a rate-versus-time or rate-versus-concentration graph can be constructed from concentration versus time data. Furthermore, if the course text is one with conceptual gaps in the introduction of the integrated rate laws, armed with the rubric presented here, instructors can readily identify and address such gaps. Students in most introductory chemistry courses will have varied calculus backgrounds: some students who are taking college calculus concurrently, some students who last had calculus in high school, and some students who are studying reaction kinetics before taking calculus. Given this diversity of experiences, it is especially important for instructors to take a learner-centered perspective to design their reaction kinetics curriculum.

Chemistry Education Researchers

In addition to contributing to the important work of bridging educational theory and classroom practice, these findings provide chemistry education researchers with guidance to develop testable hypotheses. For example, the coders in this study considered the juxtaposition of the concentration versus time and rate versus concentration multiplot graphs (see Figure 2) particularly informative, and a judicious use of textbook real estate. The juxtaposition facilitates the comparison of the shapes of the two graphs for three different reaction orders. Nevertheless, this process involves a considerable cognitive load for a novice: Do students attend to the axes? Do they follow the colors (reaction orders) from one graph to the next? Do they recognize that the slope of the first graph provides the y -coordinate for the second graph? Therefore, although Mayer's (2002) principles of multimedia learning provide general guidance for the design of pedagogically effective figures,⁵³ this study, by documenting how visualizations are commonly

used in reaction kinetics chapters, raises more specific questions about how particular visual representations, or progressions of representations, can help or hinder the development of students' understanding of rates of change concepts in reaction kinetics.

STUDY LIMITATIONS

This study has two main limitations. The first has to do with the scope of the work. By design, it is specific to reaction kinetics, and the analysis is not intended to draw inferences about the entire content of general chemistry textbooks. As such it is not a ranking or rating of textbooks. The second limitation has to do with the fact that the DBER lens is constrained by the current state of knowledge regarding students' understanding of reaction kinetics. Given the large number of student challenges with rates of change concepts and the dearth of research on how students learn from specific representations in reaction kinetics, this study (despite its systematic approach) may have missed pedagogical choices in texts that could be problematic for some learners. Thus, any relevant new findings about this area would need to be incorporated into the DBER lens.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: [10.1021/acs.jchemed.7b00238](https://doi.org/10.1021/acs.jchemed.7b00238).

Supplemental document showing the codes for each textbook in the study (PDF)

AUTHOR INFORMATION

Corresponding Author

*E-mail: sseethaler@ucsd.edu.

ORCID

Sherry Seethaler: [0000-0003-1681-4351](https://orcid.org/0000-0003-1681-4351)

Notes

The authors declare no competing financial interest.

REFERENCES

- (1) National Research Council. *Discipline-Based Education Research: Understanding and Improving Learning in Undergraduate Science and Engineering*; Singer, S. R., Nielsen, N. R., Schweingruber, H. A., Eds.; National Academies Press: Washington, DC, 2012.
- (2) Johnstone, A. H. Why Is Science Difficult To Learn? Things Are Seldom What They Seem. *J. Comput. Assist. Lear.* **1991**, *7* (2), 75–83.
- (3) Johnstone, A. H. The Development of Chemistry Teaching: A Changing Response to Changing Demand. *J. Chem. Educ.* **1993**, *70* (9), 701–705.
- (4) Murphy, K.; Holme, T.; Zenisky, A.; Caruthers, H.; Knaus, K. Building the ACS Exams Anchoring Concept Content Map for Undergraduate Chemistry. *J. Chem. Educ.* **2012**, *89* (6), 715–720.
- (5) French, M.; Taverna, F.; Neumann, M.; Paulo Kushnir, L.; Harlow, J.; Harrison, D.; Serbanescu, R. Textbook Use in the Sciences and Its Relation to Course Performance. *Coll. Teach.* **2015**, *63* (4), 171–177.
- (6) Justi, R. Teaching and Learning Chemical Kinetics. In *Chemical Education: Towards Research-Based Practice*; Gilbert, J. K., de Jong, O., Justi, R., Treagust, D., van Driel, J. H., Eds.; Springer: Netherlands, 2003; pp 293–315.
- (7) Bain, K.; Towns, M. H. A Review of Research on the Teaching and Learning of Chemical Kinetics. *Chem. Educ. Res. Pract.* **2016**, *17* (2), 246–262.
- (8) Potgieter, M.; Harding, A.; Engelbrecht, J. Transfer of Algebraic and Graphical Thinking between Mathematics and Chemistry. *J. Res. Sci. Teach.* **2008**, *45* (2), 197–218.
- (9) Seçken, N.; Seyhan, H. G. An Analysis of High School Students' Academic Achievement and Anxiety over Graphical Chemistry Problems about the Rate of Reaction: The Case of Sivas Province. *Procedia, Soc. Behav. Sci.* **2015**, *174*, 347–354.
- (10) Tuminaro, J.; Redish, E. F. Understanding Students' Poor Performance on Mathematical Problem Solving in Physics. *AIP Conference Proceedings* **2004**, *720* (1), 113–116.
- (11) Planinic, M.; Ivanjek, L.; Susac, A.; Milin-Sipus, Z. Comparison of University Students' Understanding of Graphs in Different Contexts. *Phys. Rev. ST Phys. Educ. Res.* **2013**, *9* (2), 020103.
- (12) Wemyss, T.; van Kampen, P. Categorization of First-Year University Students' Interpretations of Numerical Linear Distance-Time Graphs. *Phys. Rev. ST Phys. Educ. Res.* **2013**, *9* (1), 010107.
- (13) Gultepe, N. Reflections on High School Students' Graphing Skills and their Conceptual Understanding of Drawing Chemistry Graphs. *Educ. Sci. Theory Pract.* **2016**, *16* (1), 53–81.
- (14) Bektaşlı, B.; Çakmakci, G. Consistency of Students' Ideas about the Concept of Rate across Different Contexts. *Educ. Sci.* **2011**, *36* (162), 273–287.
- (15) Ivanjek, L.; Susac, A.; Planinic, M.; Andrasevic, A.; Milin-Sipus, Z. Student Reasoning about Graphs in Different Contexts. *Phys. Rev. ST Phys. Educ. Res.* **2016**, *12* (1), 010106.
- (16) Çakmakci, G.; Aydogdu, C. Designing and Evaluating an Evidence-Informed Instruction in Chemical Kinetics. *Chem. Educ. Res. Pract.* **2011**, *12* (1), 15–28.
- (17) Kolomuç, A.; Tekin, S. Chemistry Teachers' Misconceptions Concerning Concept of Chemical Reaction Rate. *Eurasian J. of Phys. Chem. Educ.* **2011**, *3* (2), 84–101.
- (18) Çakmakci, G.; Leach, J.; Donnelly, J. Students' Ideas about Reaction Rate and Its Relationship with Concentration or Pressure. *Int. J. Sci. Educ.* **2006**, *28* (15), 1795–1815.
- (19) McDermott, L. C.; Rosenquist, M. L.; Van Zee, E. H. Student Difficulties in Connecting Graphs and Physics: Examples from Kinematics. *Am. J. Phys.* **1987**, *55* (6), 503–513.
- (20) Beichner, R. J. Testing Student Interpretation of Kinematics Graphs. *Am. J. Phys.* **1994**, *62* (8), 750–762.
- (21) Rushton, G. T.; Criswell, B. A.; McAllister, N. D.; Polizzi, S. J.; Moore, L. A.; Pierre, M. S. Charting an Alternate Pathway to Reaction Orders and Rate Laws in Introductory Chemistry Courses. *J. Chem. Educ.* **2014**, *91* (1), 66–73.
- (22) Berry, J. S.; Nyman, M. A. Promoting Students' Graphical Understanding of the Calculus. *J. Math. Behav.* **2003**, *22* (4), 479–495.
- (23) Doerr, H. M.; Arleback, J. B. Interpreting and Communicating about Phenomena with Negative Rates of Change. *Proceedings of the 120th ASEE (American Society for Engineering Education) Annual Conference & Exposition*; Atlanta, GA, June 23–26, 2013.
- (24) Orton, A. Students' Understanding of Differentiation. *Educ. Stud. Math.* **1983**, *14* (3), 235–250.
- (25) Rowland, D. R.; Jovanoski, Z. Student Interpretations of the Terms in First-Order Ordinary Differential Equations in Modelling Contexts. *Int. J. Math. Educ. Sci. Technol.* **2004**, *35* (4), 503–516.
- (26) Bezuidenhout, J. First-Year University Students' Understanding of Rate of Change. *Int. J. Math. Educ. Sci. Technol.* **1998**, *29* (3), 389–399.
- (27) Bollen, L.; De Cock, M.; Zuza, K.; Guisasaola, J.; van Kampen, P. Generalizing a Categorization of Students' Interpretations of Linear Kinematics Graphs. *Phys. Rev. ST Phys. Educ. Res.* **2016**, *12* (1), 010108.
- (28) Orton, A. Understanding Rate of Change. *Math. Sch.* **1984**, *13* (5), 23–26.
- (29) White, P.; Mitchelmore, M. Conceptual Knowledge in Introductory Calculus. *J. Res. Math. Educ.* **1996**, *27* (1), 79–95.
- (30) Rasmussen, C.; Marrongelle, K.; Borba, M. C. Research on Calculus: What Do We Know and Where Do We Need To Go? *ZDM* **2014**, *46* (4), 507–515.

- (31) Herbert, S.; Pierce, R. What Is Rate? Does Context or Representation Matter? *Math. Educ. Res. J.* **2011**, *23* (4), 455–477.
- (32) Thompson, P. W. Images of Rate and Operational Understanding of the Fundamental Theorem of Calculus. *Educ. Stud. Math.* **1994**, *26*, 229–274.
- (33) Becker, N.; Towns, M. Students' Understanding of Mathematical Expressions in Physical Chemistry Contexts: An Analysis Using Sherin's Symbolic Forms. *Chem. Educ. Res. Pract.* **2012**, *13*, 209–220.
- (34) Thiele, R. B.; Treagust, D. F. Analogies in Chemistry Textbooks. *Int. J. Sci. Educ.* **1995**, *17* (6), 783–795.
- (35) Davila, K.; Talanquer, V. Classifying End-Of-Chapter Questions and Problems for Selected General Chemistry Textbooks Used in the United States. *J. Chem. Educ.* **2010**, *87* (1), 97–101.
- (36) Pyburn, D. T.; Pazicni, S. Applying the Multilevel Framework of Discourse Comprehension To Evaluate the Text Characteristics of General Chemistry Textbooks. *J. Chem. Educ.* **2014**, *91* (6), 778–783.
- (37) Quisenberry, K. T.; Tellinghuisen, J. Textbook Deficiencies: Ambiguities in Chemical Kinetics Rates and Rate Constants. *J. Chem. Educ.* **2006**, *83* (3), 510–512.
- (38) American Chemical Society. *Annual Reports of Earned Bachelor's Degrees in Chemistry*. <https://www.acs.org/content/acs/en/about/governance/committees/training/reports/degreesreport.html> (accessed Aug 2017).
- (39) Zumdahl, S.; DeCoste, D. *Introductory Chemistry: A Foundation*; Cengage Learning: Stamford, CT, 2015.
- (40) Atkins, P.; Jones, L.; Laverman, L. *Chemical Principles: The Quest for Insight*; W. H. Freeman and Company: New York, 2016.
- (41) Brown, T.; LeMay, H. E.; Bursten, B.; Murphy, C.; Woodward, P.; Stoltzfus, M. *Chemistry: The Central Science*; Pearson: New York, 2015.
- (42) Chang, R.; Goldsby, K. *Chemistry*; McGraw Hill Education: New York, 2016.
- (43) McMurry, J.; Fay, R.; Robinson, J. *Chemistry*; Pearson: New York, 2016.
- (44) McQuarrie, D.; Rock, P. *General Chemistry*; University Science Books: Mill Valley, CA, 2011.
- (45) Oxtoby, D.; Gillis, H.; Butler, L. *Principles of Modern Chemistry*; Cengage Learning: Boston, MA, 2016.
- (46) Silberberg, M.; Amateis, P. *Chemistry: The Molecular Nature of Matter and Change*; McGraw Hill Education: New York, 2015.
- (47) Tro, N. *Chemistry: A Molecular Approach*; Pearson: Boston, MA, 2017.
- (48) OpenStax CNX. *Chemistry*. <https://cnx.org/contents/havxkyvS@9.422:HHZ1sphc@3/Introduction> (accessed Aug 2017).
- (49) University of Texas. *Chemistry 302*. <https://ch302.cm.utexas.edu/kinetics/index.php> (accessed Aug 2017).
- (50) LibreTexts. *Chemistry*. http://chem.libretexts.org/Core/Physical_and_Theoretical_Chemistry/Kinetics/Reaction_Rates/Reaction_Rate (accessed Aug 2017).
- (51) Philipp, R. A. The Many Uses of Algebraic Variables. *Math. Teach.* **1992**, *85* (7), 557–561.
- (52) Schoenfeld, A. H.; Arcavi, A. On the Meaning of Variable. *Math. Teach.* **1988**, *81* (6), 420–427.
- (53) Mayer, R. E. Multimedia Learning. *Psychol. Learn. Motiv.* **2002**, *41*, 85–139.