CHEMICALEDUCATION

¹ Analyzing General Chemistry Texts' Treatment of Rates of Change ² Concepts in Reaction Kinetics Reveals Missing Conceptual Links

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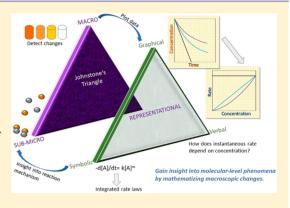
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8 Supporting Information

ABSTRACT: Change over time is a crosscutting theme in the sciences 9 that is pivotal to reaction kinetics, an anchoring concept in undergraduate 10 chemistry, and students' struggles with rates of change are well-11 documented. Informed by the education scholarship in chemistry, 12 physics, and mathematics, a research team with members from 13 complementary disciplinary backgrounds developed a rubric to examine 14 how 10 general chemistry textbooks used by top producers of American-15 Chemical-Society-approved chemistry baccalaureates treat rates of change 16 concepts in reaction kinetics. The rubric is focused on four categories of 17 students' challenges that emerged from the literature review: (i) fluency 18 19 with graphical representations, (ii) meaning of sign of rate of change, (iii) eistinction between average and instantaneous rates of change, and (iv) 20 connections between differential and integrated forms of the rate laws. 21 The analysis reveals interesting patterns but also variability among the 22



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.

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

30 **FEATURE:** Chemical Education Research

31 BACKGROUND

32 Discipline-based education research (DBER) provides consid-33 erable insight into the conceptual challenges of learning specific 34 topics. Better supporting the translation of DBER findings into 35 practice and conducting DBER at the intersection between 36 disciplines are among the recommended goals for future 37 research made by the National Research Council.¹ These two 38 goals have motivated the study described here, which uses 39 DBER as a lens to pose the following research question: How 40 do general chemistry textbooks treat rates of change concepts 41 in reaction kinetics? By "DBER as a lens" we are referring to a 42 goal-oriented, two-stage process of first examining and 43 synthesizing the literature on teaching and learning rates of 44 change, and then crafting an analytical instrument with its 45 constituent criteria directly emergent from the documented 46 challenges faced by learners. Johnstone's triangle, which 47 connects three conceptual levels of chemistry (macro, 48 submicro, representational), serves as a broad framework for

this study.^{2,3} The DBER lens developed here places particular 49 scrutiny on Johnstone's representational level. 50

The topic of this study was selected because scholarship in 51 chemistry education, physics education, and mathematics 52 education reveals widespread difficulties faced by students 53 when learning about and applying rates of change concepts. 54 The notion of change over time is fundamental to kinetics, 55 which the American Chemical Society (ACS) Examinations 56 Institute considers one of 10 anchoring concepts or "big ideas" 57 in undergraduate chemistry.⁴ Textbooks were chosen as the 58 object of study because they are required or recommended in 59 most first-year chemistry courses, and because they provide a 60 conceptual narrative that buttresses what students learn in class. 61 In a recent study of over 1000 students in a dozen introductory 62

Received: March 30, 2017 Revised: October 3, 2017



63 science courses, more than three-quarters of students reported 64 reading the textbook either often or sometimes.⁵

Reviews of the literature on teaching and learning chemical 65 66 kinetics have compiled a plethora of student difficulties and 67 misconceptions that commonly persist after instruction.^{6,7} The 68 most recent of these reviews also highlights how mathematics 69 education research on students' understanding of related rates 70 can inform this area of chemistry education.⁷ Here we drew 71 from the relevant literature in three disciplines (chemistry 72 education, physics education, mathematics education) to create 73 a list of students' rates of change challenges, which we then 74 considered in the context of introductory reaction kinetics. At 75 this intersection emerged four broad areas of student 76 difficulties: (i) drawing and interpreting graphs to understand 77 change over time, (ii) interpreting the sign in a rate of change, 78 (iii) distinguishing average and instantaneous rates of change, 79 and (iv) basic conceptual meaning behind derivatives and 80 integrals.

81 Graphical Representations

⁸² Undergraduate chemistry students have difficulty constructing ⁸³ and interpreting graphs, and may experience anxiety with ⁸⁴ chemistry problems that involve graphs.^{8,9} Graphing problems ⁸⁵ that are purely mathematical prove less difficult than problems ⁸⁶ involving the same mathematical content in a physical context ⁸⁷ that introduces the need for translation of the context into ⁸⁸ mathematical language.^{10–12} Students also face challenges when ⁸⁹ integrating process skills such as graphing and comprehending ⁹⁰ chemical events in a microworld.¹³ Because it appears ⁹¹ challenging for students to generalize the rate concept as ⁹² change over time, their interpretation of graphs is dependent ⁹³ on the domain context as well as problem format.^{14–16}

⁹⁴ When asked to sketch graphs of reaction rate versus time, a ⁹⁵ significant number of chemistry teachers produced graphs with ⁹⁶ unrealistic slopes, such as slope increasing exponentially ⁹⁷ without decreasing.¹⁷ High school students and undergraduate ⁹⁸ students also had difficulty sketching accurate reaction rate ⁹⁹ versus time graphs, even when they were able to provide ¹⁰⁰ accurate verbal descriptions of how the rate of a chemical ¹⁰¹ reaction changes over time.¹⁸ Because curved graphs involve ¹⁰² changes in both height and slope, students find them more ¹⁰³ difficult to interpret.¹⁹ Giving students the opportunity to ¹⁰⁴ predict the shapes of graphs and then compare the actual ¹⁰⁵ graphs with their predictions may be especially suited to ¹⁰⁶ 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 rate versus time graphs.¹⁸ Pollowing traditional instruction in reaction kinetics, the vast majority of first-year undergraduate students incorrectly reaction that the reaction rate versus time graph.¹⁶ The same as the concentration versus time graph.¹⁶ The reaction the relationships between graphs can rate versus for doing so.²²

118 Sign of Rate of Change

119 Studies have documented undergraduate students' difficulties 120 with negative rates of change in various contexts, including 121 kinematics (the meaning of negative velocity and negative 122 acceleration), light intensity over distance from a point source, 123 and discharge of a capacitor in a simple circuit.^{19,23} For 124 example, when determining whether something is slowing down or speeding up, students may base their responses on the 125 sign associated with the slope of the position versus time graph, 126 rather than the change in magnitude of the slope.¹⁹ They 127 struggle to attend to the magnitude or absolute value and the 128 sign of the rate of change simultaneously, and find it especially 129 confusing when rates are negative but increasing in 130 magnitude.²³ When solving equations or interpreting graphs, 131 students commonly confuse the sign of the slope with the sign 132 of the *y*-coordinate, or carelessly drop the negative sign.^{15,24} 133 These findings have implications for curricular treatment of the 134 negative sign associated with consumption of reactants.

Distinction between Average and Instantaneous Rates of 136 Change 137

Over the course of a chemical reaction, rate may remain 138 constant (zeroth-order), change linearly (first-order), or change 139 nonlinearly (second and other orders); the distinction between 140 average and instantaneous rates of change is thus central to 141 understanding relationships in reaction kinetics. Unfortunately, 142 students fail to distinguish initial rate, instantaneous rate, and 143 average rate over a time interval.¹⁸ They have difficulty saying 144 how the rate of reaction changes over time, and confound 145 constant and variable rates of change.^{7,25} A student who is able 146 to apply a procedure to calculate average rate of change may 147 not be able to explain the meaning of the average rate of 148 change.²⁶

Representationally, average and instantaneous rates of 150 change can be distinguished in words, graphically (slope of 151 the secant versus slope of the tangent), and in symbols (Δ 152 versus d), and moving between these representations presents a 153 suite of difficulties for students. Many undergraduate students 154 struggle with matching a text description with a graphical 155 representation.¹⁹ They have a poor understanding of the 156 symbol Δ .¹⁵ They may not understand that the average rate 157 equals the instantaneous rate on a linear graph.²⁷ They often 158 compute the slope at a point by simply dividing the y-value by 159 the x-value.^{19,20} They may not view the tangent as the limit of 160the set of secants.²⁸ This research demonstrates that curricular 161 support is needed to help undergraduate students develop 162 fluency with moving between these rates of change 163 representations, which are all relevant to understanding average 164 and instantaneous rates of concentration change in introduc- 165 tory reaction kinetics.

Meaning of and Connections between Derivative and Integral

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Students who have completed an introductory calculus 169 sequence still commonly treat variables as symbols to be 170 manipulated, rather than quantities to be related.²⁹ The 171 differences between high school and undergraduate are not 172 significant for the first course in differential and integral 173 calculus, although undergraduates may have further lost touch 174 with earlier mathematical knowledge and skills, such as 175 graphing, and ceased to think in terms of rate of change.^{24,30} 176 Even when students do have an understanding of rate when 177 working with one kind of representation or context, this 178 understanding does not necessarily transfer to other 179 situations.³¹

A core principle in calculus (the fundamental theorem of 181 calculus) is that the accumulation of a quantity (determined by 182 integration) and the rate of change in the accumulation of the 183 quantity (determined by differentiation) are interrelated.³² This 184 principle, of course, underlies the connection between the rate 185 laws in their differential form and in their integral form. Ideally, 186

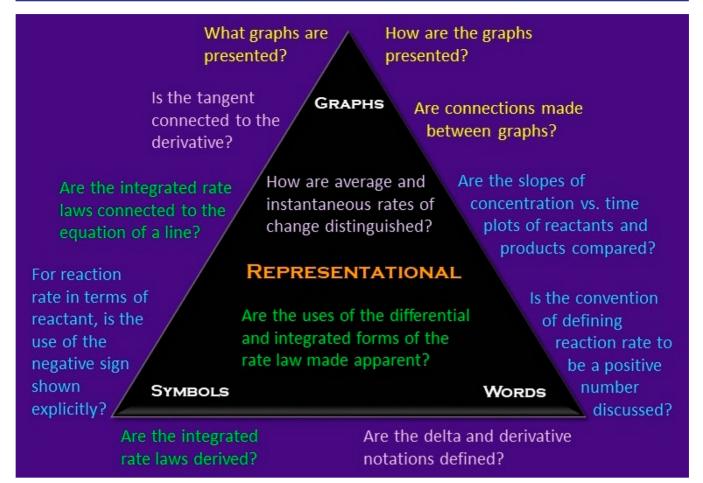


Figure 1. Supporting students to navigate the representational level of Johnstone's triangle. Color indicates the category of student difficulty: graphical representations (yellow), sign of rate of change (blue), distinction between average and instantaneous rates of change (lavender), and meaning of 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).

187 students who have studied calculus would have internalized this 188 basic idea and its implications, but this does not appear to be 189 the case. Students frequently confound "amount" and "rate of 190 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 191 192 meaning of terms in a differential equation, and mix up the 193 function and its derivative.²⁵ Relevant to integration, students 194 do not know what the area under the graph means.¹⁵ Finally, 195 students who understand the terms in y = mx + b and recognize 196 as the equation of a straight line cannot necessarily see the 197 same (y-intercept, slope) relationships when other variables are 198 involved.¹⁴ Although not strictly a calculus issue, fluency with 199 200 the equation of a line is relevant to working with the integrated 201 rate laws. These gaps in students' understanding of the 202 connections between, and conceptual meaning of, the 203 derivative and integral may not interfere with students' ability to plug and chug their way through simple kinetics problems, 204 but such a piecemeal understanding will make it difficult for 205 206 students to understand why they are doing what they are doing 207 and apply their knowledge in new contexts. Highlighting this issue, a study that examined students' ability to use calculus 209 concepts in a physical chemistry context presented a case of a 210 student who had taken six semesters of undergraduate 211 mathematics and could interpret the derivative in a

mathematics context, but could not use it to express change 212 in a thermodynamics context.³³ 213

The preceding discussion of the categories of students' 214 difficulties with rates of change concepts underlying reaction 215 kinetics underscores the particular challenges posed by the 216 representational level of Johnstone's triangle.^{2,3} In reaction 217 kinetics, various representations of macroscopic changes (i.e., of 218 concentration) are created and manipulated to gain insight into 219 molecular level phenomena (i.e., reaction mechanism). The 220 representational level can be thought of as a "triangle within a 221 triangle", involving navigation between graphical, verbal, and 222 symbolic representations. For each category of student 223 difficulty discussed above, Figure 1 shows where questions 224 fl about how texts address that area of difficulty fit within the 225 representational level. 226

Given the extensive literature on students' challenges with 227 these conceptual underpinnings of reaction kinetics, it is 228 valuable to examine to what extent textbooks make the relevant 229 connections explicit. Various studies have examined the content 230 of chemistry textbooks: documenting the analogies used to 231 explain abstract chemical concepts, creating a taxonomy of end- 232 of-chapter problems, and examining linguistic characteristics 233 and depth of cohesion of the narrative.^{34–36} One paper has 234 previously pointed out the failure of chemistry texts to clarify 235 that the rate and rate constant are ambiguous in the absence of 236 an explicit statement of the balanced reaction equation to which 237 238 they apply.³⁷ The analysis presented here contributes to the 239 research on textbooks by providing insight into the collective 240 strengths and weaknesses of textbooks in handling rates of 241 change concepts in reaction kinetics.

242 METHODS

243 **Texts**

244 The texts analyzed were the general chemistry textbooks 245 assigned by the top producers of ACS-approved chemistry 246 baccalaureates.³⁸ The textbooks used by the top 10 ACS-degree producers were all included, except one (Zumdahl), which did 247 not have a chapter on reaction kinetics.³⁹ Books by unique 248 authors used by the next five producers were also included. To 249 avoid real or perceived bias, one book by Tro (Chemistry: 250 Structure and Properties) was not scored because another text by 251 Tro was already included in the top 10. Because three 252 253 textbooks (OpenStax, Oxtoby, and Tro's Chemistry: A 254 Molecular Approach) were each represented twice on the list 255 of top 15 ACS-degree producers, the score summary includes a 256 total of 10 textbooks (referred to hereafter as Atkins, Brown, 257 Chang, McMurry, McQuarrie, Oxtoby, Silberberg, Tro, Open-Stax, UT Austin).⁴⁰⁻⁴⁹ The latter is an online text designed for 258 259 a specific course, and because its videos were core (not 260 supplemental) materials, their content was included in the 261 analysis.

262 **Raters**

263 Three raters provided insights from different disciplinary 264 perspectives. One rater was trained in chemistry (under-265 graduate and doctorate) and has taught introductory chemistry 266 extensively at the undergraduate and community college level. 267 One rater was trained in chemistry (undergraduate) and 268 science education (doctorate). One rater was trained in 269 mathematics (undergraduate and master's) and mathematics 270 education (current Ph.D. student).

271 Scoring

272 The team developed the rubric based on the literature, and 273 then iteratively refined it. The three raters independently 274 scored all the texts. Initial interrater reliability was 85% (i.e., 275 initial three-way agreement on 205 of 240 codes across the 276 texts). Discussion of the relevant narrative passages or figures 277 resolved the initial disagreements. Final interrater agreement 278 was 100%.

279 Rubric and Research Questions

280 The rubric (see Table 1) was developed to investigate texts' 281 treatment of rates of change concepts from the beginning of the 282 kinetics chapter(s), through rate expressions and the differential 283 form of the rate law, up to and including the presentation of the 284 integrated rate laws. Depending on the organization of the text, 285 this was an entire chapter, or the portion of the chapter before 286 the sections on reaction mechanism and catalysis. The rubric 287 comprised the four categories of students' challenges with rates 288 of change concepts relevant to reaction kinetics.

289 What Graphical Representations Are Used and in 290 What Ways? The finding that students have difficulty 291 predicting the shapes of rates of change graphs raises the 292 question of whether texts give students the opportunity to do 293 so. It is feasible for a textbook to include reflection prompts in 294 the flow of the narrative or in the margins, prior to the 295 introduction of fundamental graphs. The rubric asks about the 296 presence of such prompts.

Table 1. Code Summary for All Textbooks Analyzed^a

		Present?	
Rubri	c Categories and Questions Investigating the Treatment of Rates of Change Concepts in Selected Textbooks a	Yes	No
	Use of Graphical Representations to Introduce the Top	pic	
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? $^{\circ}$	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
Dis	tinction between Average, Instantaneous, and Initial Rates of	of Cha	nge
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
	codes for each individual textbook of the 10 exa	umineo numbe	

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., 297 concentration versus time, rate versus concentration, rate versus 298 time) and infer the shape of one from another, students must, 299 at minimum, be exposed to these different graphs. Thus, the 300 coding scheme documents what types of graphs are present at 301 least once in the text. Thoughtful juxtaposition of different 302 types of reaction kinetics graphs, as well as graphs alongside 303 other representations, is needed to support students' fluency of 304 movement between them. The coding scheme asks what 305 graphical representations texts juxtapose, either as separate 306 figures or via the inclusion of multiple data plots on the same 307 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	Connect the visible color change to shape of the absorption spectrum.

corresponding bromine solutions (Chang). Concentration versus time graphs for reactants and products, comparing two different Introduce the rate expression by showing that the relative rates of reactants reactions side by side (Silberberg).

How Is the Sign of Rate of Change Treated? The 309 310 positive or negative sign associated with a rate of change carries 311 meaning. In kinematics, the sign provides information about 312 direction of motion; in kinetics, the sign provides information 313 about whether a chemical species is consumed or produced. 314 Because it is clear from the literature that interpreting the sign 315 of a rate of change is troublesome for students, it is useful to examine how textbooks deal with the sign in reaction rate. The 316 317 rubric asks if the texts explain the meaning of the sign, and if 318 they make clear that the definition of reaction rate as a positive 319 quantity is a convention.

How Are Average and Instantaneous Rate Distin-320 321 guished? Because students have difficulty with the distinction 322 between rate of change over time and rate of change at one 323 point in time, and because this distinction is fundamental in 324 reaction kinetics, it is important that texts elucidate the 325 distinction between average and instantaneous rate of change, 326 ideally in words, symbols, and graphs. Recognizing initial rate of 327 change as a subcategory of instantaneous rate of change is 328 pertinent to the method of initial rates. Therefore, the coding 329 examined texts' distinction of these three rates of change 330 (average, instantaneous, initial) in the three modes of 331 presentation (words, symbols, graphs).

What Scaffolds Are Provided To Help Students 332 333 Understand and Connect the Differential and Inte-334 grated Forms of the Rate Laws? Even if students have taken 335 an introductory calculus sequence before they study reaction 336 kinetics, mathematics education scholarship demonstrates that 337 they are unlikely to have more than a rudimentary understanding of the meaning of a differential equation or integral. 338 Therefore, in introducing reaction kinetics, texts must elucidate 339 340 critical connections, such as the connection between the slope of the tangent and the instantaneous rate, and the way 341 342 integrating the differential form of the rate law brings in the variable of time. The rubric examines texts for these 343 344 connections, which can be made conceptually whether or not 345 the text is calculus-based.

RESULTS AND DISCUSSION 346

347 Graphical Representations

348 In general, the texts do not provide prompts to encourage 349 students to predict the shapes of reaction kinetics graphs, 350 although one text (Brown) partly did this in "Go Figure" and and products depend on their stoichiometric coefficients.

"Give It Some Thought" prompts, for example, showing 351 molecular depictions of reactants and products at three time 352 points and asking students to estimate the concentration at an 353 intermediary time. 354

The study revealed considerable variation in terms of what 355 graphs texts use to build up to and introduce the rate laws. On 356 one hand, all 10 texts present graphs of the following: 357 concentration (or pressure) versus time, natural logarithm of 358 concentration versus time, and inverse of concentration versus 359 time. On the other hand, only two texts (Atkins and 360 McQuarrie) present graphs of rate versus time, and only half 361 the texts present graphs of rate versus concentration. The texts 362 include a few other graph types: rate versus square of 363 concentration (Atkins), a femtosecond spectrum illustrating 364 decomposition of a halide (Atkins), plots of absorbance versus 365 wavelength for solutions at different concentrations (Brown, 366 Chang), and a bar graph showing the influence of the rate law 367 exponent on rate (McMurry).

In terms of encouraging students to move between 369 representations, the extent to which texts juxtapose two graphs, 370 or a graph and another visual, also varies. The median number 371 of juxtapositions per text is 3 (range 1-6). The most common $_{372}$ use of juxtaposition is of the characteristic integrated rate law 373 plots, with all the texts juxtaposing at least two of the three. The 374 second most common juxtaposition, present in five texts, is a 375 plot of concentration versus time with depictions of containers 376 filled with spheres, dots, or squares that represent reactant 377 concentration initially and at successive half-lives. In one text, a 378 similar graph/dot juxtaposition shows the number of reactant 379 and product molecules every 10 s. 380

Notably, in introducing the differential form of the rate laws, 381 only three texts juxtapose graphs to compare relationships 382 between concentration and time, and rate and time or 383 concentration. One text juxtaposes a graph of concentration 384 versus time with a graph of rate versus time. Two texts 385 juxtapose a graph of concentration versus time with a graph of 386 rate versus concentration. Table 2 is a compilation of 387 t2 juxtaposition types found in the 10 texts. 388

As is the case with juxtapositions, the extent to which texts 389 use the technique of comparing multiple data sets on the same 390 graph is highly variable. Median number of multiplot graphs per 391 text is 2 (range 0-5). Most common are graphs of 392 concentration versus time showing both reactants and products 393 (Chang, McMurry, McQuarrie, Silberberg, Tro, OpenStax); 394

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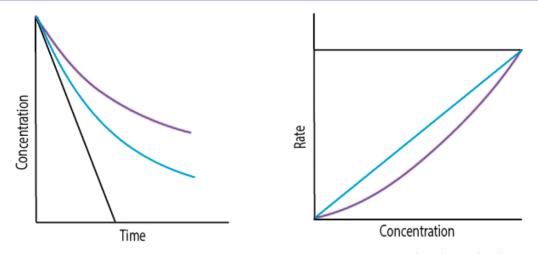


Figure 2. Juxtaposition of graphs of concentration versus time and rate versus concentration for a zeroth- (black), first- (blue), and second- (purple) order reaction.

395 another text shows reactants and products on a femtosecond 396 spectrum (Atkins). Four texts compare plots for different 397 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 399 (Atkins); concentration versus time for a zeroth-, first-, and 400 second-order reaction (Silberberg and Tro); and rate versus 401 402 concentration for a zeroth-, first-, and second-order reaction 403 (Silberberg and Tro). Figure 2 juxtaposes these two latter 404 multiplot graphs, as presented in Silberberg and Tro. Only one 405 other multiplot figure appears in more than one text: 406 absorbance versus wavelength for different concentrations 407 (Brown, Chang). One text (Atkins) presents three multiplot 408 graphs not used by other texts: concentration versus time for 409 various initial reactant concentrations, concentration versus 410 time for several rate constants, and ratio of current to initial 411 reactant concentration versus time to show dependence of half-412 life of a first-order reaction on the rate constant.

413 Sign of Rate of Change

414 When introducing the rate expression, all the texts point out 415 that the rate of concentration change of a reactant is negative. 416 All but one (Oxtoby) indicate that a negative sign is added to 417 make the rate of reaction a positive quantity. Six of the texts 418 (Atkins, Brown, McMurry, Silberberg, Tro, OpenStax) point 419 out that this is a convention (or because rate of reaction is 420 defined as a positive quantity). None of the 10 texts scored here 421 stated or suggested that the negative sign does not make sense; 422 however, a statement to this effect was noted in another online 423 text:⁵⁰

- 424 Since negative rates do not make much sense, rates expressed
- 425 in terms of a reactant concentration are **always** preceded by
- 426 a minus sign to make the rate come out positive.
- 427 Average and Instantaneous Rate

428 **Words.** All the texts except one (UT Austin) distinguish 429 average, instantaneous, and initial rates of change using words. 430 The texts, except three (Tro, UT Austin, OpenStax), also 431 explain the difference between the tangent and the secant in 432 terms of the time interval being considered.

Graphs. Three texts (Atkins, McMurry, Silberberg) use tage graphs to distinguish average, instantaneous, and initial rates. Two texts (McQuarrie, Oxtoby) distinguish average and instantaneous (but not initial) rates graphically, and two texts tage (Brown, OpenStax) distinguish instantaneous and initial (but not average) rates graphically. The remaining three texts do not 438 use graphs to distinguish the different kinds of rates. 439

Symbols. All the texts use the delta (Δ) notation. Four texts 440 (McMurry, McQuarrie, Silberberg, OpenStax) do not use the 441 derivative (d) notation; however, of the texts that use the Δ 442 and d notation, only three (Atkins, Brown, Oxtoby) defined 443 both notations. The remaining three texts (Chang, Tro, UT 444 Austin) use both notations without defining them. 445

Differential and Integrated Forms

In terms of the use of calculus in introducing the integrated rate 447 laws, the texts examined fell into three categories: narrative 448 presenting integrated rate laws without deriving them (Brown, 449 McMurry, McQuarrie, Silberberg, OpenStax), integration 450 shown as an aside in margin (Chang, Tro), and integration 451 central (Atkins, Oxtoby, UT Austin). Presence or absence of 452 calculus steps, however, does not predict a text's treatment of 453 the relationship between the tangent and the derivative. Only 454 three texts, two of which are calculus-based (Atkins and 455 Oxtoby) and one of which presents no calculus (Brown), 456 explicitly state the connection between the tangent and the 457 derivative. Another text (OpenStax) mentions that calculus is 458 used to evaluate the slope of tangent lines. The connection 459 between the tangent and the derivative, and the difficulty of 460 finding the tangent by hand, can help establish the need for the 461 integrated rate laws. As stated in Atkins (p 592) 462

Because it is difficult to draw a tangent accurately by eye, it is463better to use a computer to analyze graphs of concentration464against time. A superior method—which is described in465Topic 7B [Integrated Rate Laws]—is to report rates using a466procedure that, although based on these definitions, avoids467the use of tangents altogether.468

For the most part, the texts fail to provide this chain of logic, 469 and two texts (Brown, Chang) calculate the slope of the 470 tangent using the rise over run calculation (the same as they use 471 for calculating the slope of the secant), without mentioning that 472 doing so by eye is error prone. Overall, the texts did a better job 473 of explaining what one can learn from the integrated rate laws, 474 with reference to the variable of time, and reminding students 475 about the equation/graph of a straight line in connection to the 476 integrated rate laws. 477

Two additional aspects of the texts' mathematics coverage 478 deserve mention. The first concerns the meaning of symbols. 479 The coder with the mathematics/mathematics education 480 481 background noted that students may not have encountered the 482 proportionality (\propto) symbol or the double inequality (\gg) 483 symbol in lower division mathematics classes, and furthermore, 484 these symbols may have different meanings in other contexts. 485 Along with the observation that some texts use the derivative 486 notation without defining it, this underscores the importance of 487 defining symbols.

488 The second aspect of the texts' mathematics coverage 489 concerns mathematical integrity. Most of the texts that 490 presented the integrated rate laws use single variables in 491 multiple ways within an individual definite integral. This stood 492 out to the coder from the mathematics/mathematics education 493 background (but not to the coders from chemistry back-494 grounds, 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 ⁴⁹⁵ upper limit of integration \int_0^c , a variable in the integrand $\frac{1}{c^2}$, and ⁴⁹⁷ the variable of integration *dc* (similarly for the *t* on the right ⁴⁹⁸ side of the equation). Mathematicians distinguish between the ⁴⁹⁹ limits of integration and the variables of integration. For ⁵⁰⁰ example, they may write the above equation as

 $\int_{0}^{c_{t_1}} \frac{1}{c^2} dc = -2k \int_{0}^{t_1} dt, \text{ or simply use different variables for}$

501 the limits of integration. To do otherwise muddles the 502 distinction between values and variables, another area the 503 mathematics education literature points to as a source of 504 difficulty for students.^{51,52}

505 IMPLICATIONS

506 The decisions made by curriculum designers may be conscious 507 or unconscious. Writing a textbook involves conscious trade-508 offs between pedagogy and practicality due to publishers' 509 limitations on length, layout, number of figures, and available 510 color palette; moreover, in omitting or including calculus 511 derivations, textbook authors are making conscious choices to 512 appeal to specific audiences. Similarly, the author of every 513 textbook in this study recognized the need to explicitly connect 514 y = mx + b with the integrated rate laws. Texts also had 515 explanations about logarithms and exponents; one even 516 included a figure to help students visualize how changing the 517 exponent in the differential form of the rate law affects the 518 reaction rate.

Yet, the most powerful aspect of the DBER lens is not in s20 assessing these conscious choices to help students negotiate the s21 representational level, but in revealing unconscious decisions. s22 By definition, the DBER lens places the learner's understanding s23 of a topic at the center of the analysis. Viewed from the s24 learner's perspective, "adding in" a negative sign to make the s25 rate of disappearance of reactant a positive quantity is puzzling s26 and at odds with students' prior mathematics experience. It is s27 unlikely to be a conscious pedagogical choice that some texts s28 lacked a clear statement that this practice is a convention to s29 express reaction rate equivalently for reactants and products.

Likewise, conceptual connections necessary to help students times from the differential form of the rate law to the integrated trate laws are often unconsciously glossed over, including the following: the graphical distinction between average and times are of change, visual depictions of how the the sist reaction rate changes over time or concentration, the limitation for the rise over run slope calculation, and the relationship between the derivative and the tangent. These choices are not the calculus level of the text. For example, the non-calculus-based OpenStax textbook explains that calculus is 539 needed to determine the slope of the tangent; in contrast are 540 the texts that unproblematically calculate the slope of the 541 tangent using rise over run. The DBER lens thus highlights 542 where reaction kinetics instructional materials neglect the 543 learner-centered perspective, which may inadvertently encour- 544 age rote learning and seed the prevalent postinstruction 545 misconceptions documented in the literature. 546

These findings also provide actionable insights for chemistry 547 instructors and chemistry education researchers. 548

Chemistry Instructors

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Many factors, including cost, influence textbook choice, and 550 individual instructors may not be free to choose the course 551 textbook when the decision is made at the departmental level. 552 This study provides criteria to help instructors "troubleshoot" 553 their textbooks, and design lessons and select supplemental 554 course materials to complement the text. DBER recommends 555 that students be given the opportunity to predict the shapes of 556 graphs and compare their predicted graphs with actual data, but 557 textbooks do not provide this opportunity. Instructors could 558 address this through small group work or clicker questions with 559 whole class discussion, by having students sketch graphs or 560 select from multiple-choice options and explain their choice. 561 For example: 562

- Which of these graphs do you think best depicts how the 563 concentration of the reactant will decrease over time: 564 linear decrease, sharply decreasing slope that levels off, or 565 level slope that subsequently drops off more rapidly? 566
- What do each of these graph shapes mean about the 567 progress of the reaction? (See also ref 21.) 568

Similarly, instruction can delve into how a rate versus time or 569 rate versus concentration graph can be constructed from 570 concentration versus time data. Furthermore, if the course text 571 is one with conceptual gaps in the introduction of the 572 integrated rate laws, armed with the rubric presented here, 573 instructors can readily identify and address such gaps. Students 574 in most introductory chemistry courses will have varied calculus 575 backgrounds: some students who are taking college calculus 576 concurrently, some students who last had calculus in high 577 school, and some students who are studying reaction kinetics 578 before taking calculus. Given this diversity of experiences, it is 579 especially important for instructors to take a learner-centered 580 perspective to design their reaction kinetics curriculum. 581

Chemistry Education Researchers

In addition to contributing to the important work of bridging 583 educational theory and classroom practice, these findings 584 provide chemistry education researchers with guidance to 585 develop testable hypotheses. For example, the coders in this 586 study considered the juxtaposition of the concentration versus 587 time and rate versus concentration multiplot graphs (see Figure 588 2) particularly informative, and a judicious use of textbook real 589 estate. The juxtaposition facilitates the comparison of the 590 shapes of the two graphs for three different reaction orders. 591 Nevertheless, this process involves a considerable cognitive load 592 for a novice: Do students attend to the axes? Do they follow the 593 colors (reaction orders) from one graph to the next? Do they 594 recognize that the slope of the first graph provides the y- 595 coordinate for the second graph? Therefore, although Mayer's 596 (2002) principles of multimedia learning provide general 597 guidance for the design of pedagogically effective figures, 53 598 this study, by documenting how visualizations are commonly 599

600 used in reaction kinetics chapters, raises more specific questions 601 about how particular visual representations, or progressions of 602 representations, can help or hinder the development of 603 students' understanding of rates of change concepts in reaction 604 kinetics.

605 **STUDY LIMITATIONS**

606 This study has two main limitations. The first has to do with 607 the scope of the work. By design, it is specific to reaction 608 kinetics, and the analysis is not intended to draw inferences 609 about the entire content of general chemistry textbooks. As 610 such it is not a ranking or rating of textbooks. The second 611 limitation has to do with the fact that the DBER lens is 612 constrained by the current state of knowledge regarding 613 students' understanding of reaction kinetics. Given the large 614 number of student challenges with rates of change concepts and 615 the dearth of research on how students learn from specific 616 representations in reaction kinetics, this study (despite its 617 systematic approach) may have missed pedagogical choices in 618 texts that could be problematic for some learners. Thus, any 619 relevant new findings about this area would need to be 620 incorporated into the DBER lens.

621 ASSOCIATED CONTENT

622 **Supporting Information**

623 The Supporting Information is available on the ACS 624 Publications website at DOI: 10.1021/acs.jchemed.7b00238.

625 Supplemental document showing the codes for each 626 textbook in the study (PDF)

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632 Notes

633 The authors declare no competing financial interest.

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