Where is Calculus in Chemistry? Determining Content Alignment Between Calculus and Chemistry

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Previous research indicates that mathematics ability predicts student success in chemistry courses. Not surprisingly, chemistry students are required to take courses in mathematics as prerequisites and co-requisites, including calculus. In this work, we seek to identify the ways calculus skills and concepts appear in the undergraduate chemistry curriculum, focusing on the introductory general chemistry sequence. To this end, we combined relevant disciplinary frameworks and looked for alignment: the Calculus Content Framework (CCF) and the Anchoring Concepts Content Map (ACCM) for general chemistry. Preliminary results indicate explicit use of calculus is not common in introductory chemistry, although there are opportunities for instructors to use the general chemistry topic of chemical kinetics as a context for the application of differentiation and integration. Future work will involve mapping out the landscape of the remainder of the undergraduate chemistry curriculum and as an expected outcome of this work we seek to provide tangible resources to facilitate cross-disciplinary discussions between instructors in calculus and chemistry.

Keywords: Calculus, Chemistry, Curriculum Analysis, Interdisciplinary

Introduction

There is a large body of literature that indicates students' mathematical ability correlates with success in chemistry courses (Bain et al., 2014; Becker & Towns, 2012; Derrick & Derrick, 2002; Hahn & Polik, 2004; House, 1995; Nicoll & Francisco, 2001; Spencer, 1996; Tsaparlis, 2007; Wagner et al., 2002), which is not surprising given the large role mathematics plays in typical chemistry courses (Stowe et al., 2021). That said, student performance on standardized mathematics assessments (e.g., SAT) is often used to identify at-risk students and identify particularly challenging chemistry topics (Lewis & Lewis, 2007; Ralph & Lewis, 2018). Based on the emphasis placed on mathematics as a tool to explain and predict in chemistry, it is not uncommon to have prerequisite and co-requisite calculus courses for undergraduate students taking chemistry. For example, at the University of Wisconsin – Milwaukee, chemistry majors are required to take three semesters of calculus (covering topics including limits, derivatives, integrals, partial derivatives, and vectors), with the recommendation (not requirement) to take a course focusing on linear algebra and differential equations("Chemistry Major," 2024). However, there is a need to evaluate the alignment between the mathematics used in chemistry courses and the mathematics presented in calculus courses. To this end, we are interested in mapping the calculus concepts (Sofronas et al., 2011) on to chemistry concepts (Murphy et al., 2012).

In broad strokes, this project is the result of an interest in developing resources that further interdisciplinary connections and continue the on-going dialogue regarding how disciplines such as chemistry and mathematics can support one another to improve teaching and learning. Recently the authors attended *The Learning and Teaching of Calculus Across Disciplines* conference in Bergen, Norway (*Welcome*, 2023). The aim of this interdisciplinary conference was to bring researchers from multiple fields (biology, chemistry, economics, engineers, physicists) together to discuss how each discipline uses calculus concepts. The current preliminary report builds on a plenary talk given by Dr. Brian Faulkner at this conference that discussed prior work involving analyzing where calculus concepts are used in an engineering course (Faulkner et al., 2020), with Faulkner's work mirroring a study in mathematics that analyzed the role of calculus concepts in an advanced mathematics course (Czocher et al., 2013). Focusing on connections between chemistry and calculus communities, the intended outcome of this work is a practical tool for calculus instructors to see the contexts and extent calculus is used across the undergraduate chemistry curriculum to inform instructional choices. The guiding research question addressed in this report is, *Which concepts and skills learned in calculus are applied in general chemistry?*

Disciplinary Frameworks

The scope of this study is supported by readily accessible disciplinary-specific frameworks that outline the target content goals for chemistry (Murphy et al., 2012) and calculus (Sofronas et al., 2011). In the case of chemistry, the American Chemical Society Exams Institute developed the Anchoring Concepts Content Map (ACCM), which was developed through workshops with content experts (Murphy et al., 2012). There is currently an ACCM for the following chemistry course sequences in the undergraduate chemistry curriculum: general chemistry (Holme et al., 2015); organic chemistry (Raker et al., 2013); inorganic chemistry (Marek et al., 2018); physical chemistry (Holme et al., 2018); and analytical chemistry (Holme et al., 2020). The general multi-tiered structure for each ACCM involves a series of nested concepts that become increasingly more specific: big idea (also called anchoring concept), enduring understanding, subdisciplinary articulation, and content detail. For each ACCM, the big idea and enduring understanding levels reflect broad concepts that are relevant throughout the chemistry curriculum, whereas the subdisciplinary articulation and content detail levels are specific to individual courses (or course sequences), such as general chemistry or organic chemistry. Within the ACCM framework, there are ten big ideas, one of which is *Kinetics*. To illustrate the structure of the ACCM, the levels from the general chemistry ACCM are provided related to the *Kinetics* big idea (Holme et al., 2015):

1. Big Idea. Kinetics: Chemical changes have a time scale over which they occur.
2. Enduring Understanding. Chemical change can be measured as a function of time and occurs over a wide range of time scales.
3. Subdisciplinary Articulation. The rate of the reaction must be defined in a manner that is not dependent on which reactant or product is used to measure it.
4. Content Detail. The reaction rate should incorporate reaction stoichiometry when it is defined.

In the case of describing the calculus concepts, this study utilizes the Calculus Content Framework (CCF) (Sofronas et al., 2011). The CCF was developed through interviewing experts in the calculus field, including prominent textbook authors, experienced educators, and researchers. The focus of the interview questions was to elicit instructional goals for students in a first-year calculus sequence. To this end, the resulting CCF is organized based on four broad categories: (a) mastery of the fundamental concepts and/or skills of the first-year calculus; (b) construction of connections and relationships between and among concepts and skills; (c) the ability to use the ideas of the first-year calculus, and (d) a deep sense of the context and purpose of the calculus. Prior work has illustrated the utility of the CCF, with Czocher et al. (2013) applying the framework to investigate the necessary calculus content and skills in an advanced mathematics course and Faulkner et al. (2020) doing the same for an engineering course. In both cases, the researchers found a lack of alignment across courses, suggesting the need to consider not just whether calculus is used in future coursework, but also how calculus is used.

Methods

Data Collection & Analysis

To map calculus topics to chemistry, we focused on the *subdisciplinary articulation* level within the general chemistry ACCM, which typically represents a two-semester course sequence for first-year students. This was compared to the calculus concepts and skills developed in the CCF (*mastery of the fundamental concepts and/or skills of the first-year calculus*, discussed above). Our approach for this report is based on the methods described by (Czocher et al., 2013) and (Faulkner et al., 2020), which involved attending to mathematics-in-use to assess where and how the calculus appears in general chemistry. Using the mathematics-in-use technique requires analyzing the chemistry content (as described in the subdisciplinary articulation of the ACCM) and noting the ways calculus concepts and/or skills are involved by solving problems associated with the subdisciplinary articulation. As part of this, it is helpful to assess secondary routes that are available to solve the problem which often results in situations where calculus skills and concepts are an available route to successfully solve the problem, but another route is favored. To this end, the subdisciplinary articulations were evaluated based on whether: (0) there was no calculus associated with the related concepts and skills; (1) calculus was present, but it was not the preferred method to solve related problems and reason through and the concepts; (2) the application of calculus was the preferred approach toward solving problems and reasoning through the concepts. For this work, we report on our analysis related to the subdisciplinary articulations that fall nested under the ten big ideas in the general chemistry ACCM.

Preliminary Results

Our preliminary analysis, shown that the only calculus concept or skill present in general chemistry is derivatives. The subdisciplinary articulations that involve this concept are shown in Table 1. The only big idea from the ACCM that involved calculus concepts and skills (derivative) was chemical kinetics, which had three subdisciplinary articulations characterized as having calculus present, but not as the preferred approach. The remainder of the subdisciplinary articulations across the ten big ideas in the general chemistry ACCM did not involve calculus concepts and skills.

Table 1. ACCM subdisciplinary articulations involving derivatives.

The rate of the reaction must be defined in a manner that is not dependent on which reactant or product is used to measure it.
Rate is generally defined as the change in concentration of a reactant or product as a function of time.
When solids are included in reactions, surface area is an important factor in the rate of reaction.
Laboratory observation of reaction rates helps to establish the concept of reaction time scales empirically.

Chemical kinetics involves modeling the rate of a reaction to track changes in the concentration of reactants as a function of time. Thus, although chemical kinetics could readily be modeled using the derivative, this perspective is often circumvented in a first-year chemistry course. In the chemistry curriculum, topics are often explained with less rigorous mathematics detail, and subsequently revisited in upper-level courses. For example, one subdisciplinary articulation that was coded as having an alternative calculus explanation available was: “Rate is generally defined as the change in concentration of a reactant or product as a function of time.” In first-year general chemistry courses, the rate of a simple reaction ($A + B \rightarrow AB$) is typically defined as:

$$rate = k[A]^m[B]^n \tag{1}$$

Here, *rate* is the rate of the reaction, *k* is the rate constant, *m* and *n* are empirically determined reaction orders that describe the concentration dependence of rate, and the final equation is known as the *rate law*. This is the most common way to discuss chemical kinetics with introductory students, without associating the equation with derivatives. With this version of the rate law, students are expected to determine the reaction order, solve for the value of *k,* and generally, use algebra computational skills to manipulate variables and compute values.

In contrast, in upper-level courses such as physical chemistry, the rate law would be discussed using the differential form:

$$-\frac{d[AB]}{dt} = k[A]^m[B]^n \tag{2}$$

In the case, we make use of calculus to describe the rate of the reaction to afford a more complicated analysis of chemical systems. Often, the rate law for a reaction is integrated to further describe reactions (Table 2). The integrated rate law is helpful because the rearranged linear form of the integrated rate law can be used in laboratory contexts to determine reaction order by fitting kinetics data and assessing its agreement with the equations for each reaction order.

Table 2. Summary of equations corresponding to each reaction order.

	First-Order Reaction	**Second-Order Reaction**	**Zero-Order Reaction**
Chemical Reaction	$A \rightarrow B$	$2A \rightarrow B$	$A \xrightarrow{catalyst} B$
Rate Law	$rate = \frac{-d[A]}{dt} = k[A]^1$	$rate = \frac{-d[A]}{dt} = k[A]^2$	$rate = \frac{-d[A]}{dt} = k[A]^0 = k$
Integrated Rate Law	$-\int_{[A]_0}^{[A]} \frac{d[A]}{[A]} = k\int_0^t dt$	$-\int_{[A]_0}^{[A]} \frac{d[A]}{[A]^2} = k\int_0^t dt$	$-\int_{[A]_0}^{[A]} d[A] = k\int_0^t dt$
	$\ln\frac{[A]_0}{[A]} = kt$	$\frac{1}{[A]} - \frac{1}{[A]_0} = kt$	$[A] - [A]_0 = -kt$
Linear	$\ln[A] = -kt + \ln[A]_0$	$\frac{1}{[A]} = kt + \frac{1}{[A]_0}$	$[A] = -kt + [A]_0$

Conclusion and Questions

Within the first-year general chemistry course, calculus concepts and skills are not prominent, with the relevant mathematics required being related to other mathematics courses (e.g., algebra). This is not to suggest that calculus concepts and skills are not relevant for modeling phenomena in chemistry, but that calculus becomes more important in undergraduate chemistry courses as students advance to higher coursework. As an implication, we highlight that although calculus is often a prerequisite or corequisite for students in introductory chemistry courses, students struggling with the mathematics in chemistry need additional support and practice with mathematics at the pre-calculus level. Regarding future work, as part of the ongoing analysis, we are interested in expanding our focus toward the ways calculus concepts and skills are used across the rest of the undergraduate chemistry curriculum. Especially in upper-level chemistry courses such as physical chemistry in which calculus is heavily integrated through the curriculum. Moreover, our goal is for this work to be helpful to connect the mathematics and chemistry communities by discussing how we use the shared language of calculus. For the scope of this conference report, we have some general questions for the mathematics community:

1. What are some of the ways chemistry instructors and chemistry education researchers can support mathematics instructors and researchers interested in undergraduate mathematics education?
2. What suggestions do you have regarding the methodological approach and scope of this work?

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