APPLIED MATHEMATICS FOR CHEMISTRY MAJORS

Rachel Neville[1], Amber T. Krummel[2], Nancy E. Levinger[2], Patrick D. Shipman[3]
[1] University of Arizona, Department of Mathematics, Tucson, Arizona, United States;
[2] Colorado State University, Department of Chemistry, Fort Collins, Colorado, United States
[3] Colorado State University, Department of Mathematics, Fort Collins, Colorado, United States;

Abstract

The math that chemistry students need is significant. In physical chemistry, students need to be comfortable with ordinary and partial differential equations and linear operators. These topics are not traditionally taught in the calculus sequence that chemistry students are required to take at Colorado State University, thus mathematics can present a significant barrier to success in physical chemistry courses. Through the collaboration of the mathematics and chemistry departments, Colorado State University has developed and implemented a two-semester sequence of courses, Applied Mathematics for Chemists (MfC), aimed specifically at providing exposure to the math necessary for chemistry students to succeed in physical chemistry. The prerequisite for the sequence is a first semester of Calculus for Physical Scientists—that is, a working knowledge of derivatives, integrals and their relation through the Fundamental Theorem of Calculus. MfC begins with a look at the Fundamental Theorem of Calculus that emphasizes a scientific realization that it provides, namely an understanding of physical phenomena in terms of an initial condition and the rate of change. This introduces the first topic of MfC, namely first- and then second-order differential equations. Working with differential equations at the start of the course allows for questions from chemistry to motivate the mathematics throughout the sequence. Solving the differential equations naturally introduces students to another fundamental mathematical concept for physical chemistry, and another theme of the course, namely linear operators. The flow of the course allows for topics traditional to second and third semesters of calculus, such as Taylor series and complex numbers, to be motivated by solving chemical problems and leads to some topics, such as Fourier series, which are not part of the standard calculus sequence. Feedback from students who have taken MfC and then physical chemistry has been positive.

Keywords: Physical Chemistry, Undergraduate Curriculum, Interdisciplinary Curriculum, Linear Operators

Introduction

The depth and breadth of mathematical skills that chemists need is significant. Like most American college and university chemistry curricula leading to the BA or BS degree, Colorado State University (CSU) has previously required students complete three semesters of calculus. This more than fulfills the requirements for the ACS approved chemistry degree (ACS, 2015). However, these calculus courses omit mathematical topics such as differential equations and linear operators that are imperative for understanding physical chemistry. Similarly, the traditional calculus courses like those at CSU, cover content such as a broad range of integration techniques that are not of immediate use in physical chemistry. From the instructors' perspective, the chemistry major would require students to take significantly more mathematics, including linear algebra and differential equations, prior to taking physical chemistry. However, requiring these math courses would add credits to the chemistry major that already requires a lot of classes, making the curriculum less flexible and potentially decreasing the number of students majoring in chemistry.

To provide chemistry students with appropriate mathematical background, and to refresh topics that students may have forgotten since their last math course, some CSU chemistry instructors have offered a "just-in-time math review" as an addendum to the Physical Chemistry 1 course. Because it is optional, not all students enrolled in the math review, reducing its potential impact. To address the mismatch between the required calculus courses and to provide a math curriculum more aligned with the needs of chemistry courses, we have developed a two-semester math sequence, Applied Math for Chemists I and II (MATH 271 and 272) at CSU.

Motivation and Background

Among students at CSU and elsewhere, physical chemistry has the reputation of being a very challenging course. Derrick and Derrick studied success of students at Valdosta State University and suggest that the "formidable perception" of physical chemistry is due to the mathematical and conceptual difficulty rather than the chemistry itself (Derrick & Derrick, 2002). Early attempts to identify students who would struggle in a physical chemistry course resulted in a diagnostic quiz that tests students' background in mathematical concepts deemed necessary for physical chemistry (Porile, 1976).

Prior success in math courses significantly impacts a student's success in physical chemistry. For instance, Hahn and Polik showed that student success in physical chemistry correlate significantly both with the amount of mathematics that a student has taken and grades earned in these mathematics courses (Hahn & Polik, 2004). Instructors at CSU have observed the same trend. In another study surveying instructors of physical chemistry courses across several hundred universities, 61% of instructors indicated that students struggle because they lack the necessary mathematical background and a third of instructors reported that students do not make connections between physical chemistry concepts and the mathematics on which those concepts are based (Fox & Roehring, 2015). This suggests that not only the mathematical concepts, but also their connections to chemistry are important to student success. In fact, after lengthy conversations with colleagues, one professor concluded "College students in the sciences often grasp the operations of mathematics but miss the connection between mathematical operations and the physical systems they describe." (DeSieno, 1975) Given these observations, it seems that we could provide a better math background to help our students succeed in physical chemistry.

In 2000, the Mathematical Association of America (MAA) organized a series of Curricular Foundations Workshops to seek input on mathematics curriculum from chemists, biologists, physicists, and engineers whose students rely on a strong foundation in mathematics (Craig, 2001). Various working groups developed recommendations regarding the mathematical skills necessary for students in specific fields. A working group composed of chemistry and mathematics faculty from different institutions gave a thorough recommendation of the content and conceptual principles that students should be taught and a recommendation for the division of responsibility (see table in the appendix of (Craig, 2001)).

Several topics were given high priority for mathematics competence of students in the chemical sciences, namely multivariate calculus, creating and interpreting graphs, spatial representations and linear algebra. Nearly all relations that students will encounter in chemistry contexts are multivariate. Therefore, students should be comfortable with handling multivariate problems, thinking of variables as more than merely a spatial extent or time. Due to large variations in physical scale of problems, students should be able to decide if solutions are reasonable with estimation techniques and order of magnitude calculations. There should also be an emphasis in visualizing structures in three dimensions.

The course sequence at Colorado State University was initiated by a request by faculty members in the Department in Chemistry who were seeking ways to improve student performance in the two-semester, upper-division undergraduate course in physical chemistry. These faculty members believed that deficiency in mathematical preparedness presented a significant barrier to student success, both in terms of the mathematical topics covered in the prerequisite courses (a standard three-semester calculus sequence covering topics through multivariate calculus and targeting students in physical sciences and engineering) and student ability to apply the mathematical topics covered in those courses in their chemistry courses. Faculty members from the Departments of Chemistry and Mathematics collaborated to design the sequence of two 4-credit, semester-long courses, called *Applied Mathematics for Chemists* (MfC). The sequence was taught as an experimental course in the academic years 2014-2015 and 2015-2016 (with temporary course numbers, standard at CSU) and was accepted into curriculum of the Mathematics Department and as a prerequisite for the physical chemistry sequence in 2016 (course numbers MATH 271 and MATH 272).

Course Content

MfC has a prerequisite of Calculus for Physical Scientists 1 (derivatives and integrals) and serves as the mathematics prerequisite for the physical chemistry course. While there is some necessary mathematical background required for other chemistry courses, physical chemistry has the highest mathematical demands. The goal of the MfC courses is to provide students with a working proficiency of the mathematics so that they can focus on learning and understanding the chemistry.

Two texts are used for MfC, namely Enrich Steiner's *The Chemistry Maths Book* (Steiner, 2007), and Donald McQuarrie's *Mathematics for Physical Chemistry* (McQuarrie, 2008). Both books focus specifically on mathematical topics relevant to chemists. These texts take a practical, straightforward approach, with less emphasis on theory or proofs of theorems and more emphasis on developing a student's mathematical tools applied to practical problems. The texts cover similar material, but the Steiner book is more complete mathematically, whereas the McQuarrie book has more detail on connections with physical chemistry. Students appreciated the full solutions freely available on the publisher's website for *The Chemistry Maths Book*, as it offered quick feedback and an opportunity for individual practice. *Mathematics for Physical Chemistry* is written by the same author as the text that is used in the physical chemistry course at CSU and expands on math review sections that are included in the chemistry text (McQuarrie, 2008).

Clear recommendations for mathematics courses for chemistry majors were given in the MAA Curricular Foundations Workshops (Craig, 2001), specific to the chemistry context. The expectation is set that math courses should develop 14 conceptual principles, nearly all of which are addressed in MfC. The exceptions are an extensive discussion of numerical methods, representation of information as analog or digital, statistics and curve fitting. Statistics and regression are covered in a statistics course that chemistry students are also required to take. All principles are marked in two categories, (1) they should be developed by mathematicians, and (2) the teaching of the mathematical concept in the specific context of chemistry is particularly effective. The material covered in this course is substantial, though necessary for the future success of chemistry students.

The course is topically divided into five parts. Parts 1 (differential equations, series, and complex variables) and 2 (linear algebra), are covered in the first semester. The second semester covers parts 3 (inner product spaces and Fourier series), 4 (multivariable calculus), and 5 (partial differential equations).

The highlight in the prerequisite course (one semester of The Calculus) is the Fundamental Theorem of Calculus (FTC), typically written as

$$f(b) - f(a) = \int_a^b f'(s)ds.$$

Students see two interpretations of this relation. With *s* equal to a spatial variable *x*, the FTC gives an area underneath the graph of $f'(x)$ in the domain $a \leq x \leq b$. With *s* equal to time *t*, the FTC gives the total change in f over the time interval $a \leq t \leq b$. But, honestly, why calculate the total change $f(b) - f(a)$ by some complicated integral? MfC opens with a slight but tremendously revealing rewriting of the FTC;

$$f(t) = f(0) + \int_0^t f'(s)\, ds.$$

Any differentiable function $f(t)$ can be written in terms of an initial condition $f(0)$ and a rate of change $f'(t)$. This mathematical insight also opens up a whole new way of thinking scientifically and leads into the first part of MfC, namely ordinary differential equations. We cover chemical basic first- and second-order linear homogeneous and inhomogeneous differential equations and solution methods such as separation of variables, integrating factors, and the method of undetermined coefficients. Applications in chemical kinetics, the harmonic oscillator and a first look at Schrödinger's equations for a particle in a box motivate each class of equations. Complex numbers and series are taught as necessary theory for working with more complex systems. The grand finale of the unit on ordinary differential equations is the method of using power series to solve differential equations. Chemistry students are typically not exposed to these mathematical topics because they comprise topics in an ordinary differential equations course, which is not required for chemistry majors.

Part 2 covers linear algebra. Students are introduced to vectors and are encouraged to think of vectors as coordinates in physical space as well as holding variables that are not necessarily distance. There is an emphasis on what insights determinants and eigenvalues give when modeling a physical system. Symmetries and group axioms are taught primarily through linear transformations, with some discussion on finding group representations. Compelling examples come from symmetries of planar molecules (Hückel molecular orbital method) and distributions of electrons in p-orbitals. Several students reported this application as being the most compelling example from the entire course.

The second semester and Part 3 of MfC begins with the notion of a vector space and a basis. As inner product spaces are introduced, parallels are drawn between finite-dimensional vector spaces and infinite-dimensional inner product spaces. This gives students a concrete footing in a topic that they find very theoretical. Orthogonal polynomials (including special sets of polynomials) are introduced. Rather than emphasizing the (often fairly involved) derivation of these polynomials, students are challenged to understand them as a basis for modeling specific physical systems. This notion is initiated here and developed further in the end-of-the-year project. Finally, students learn Fourier series and work with Fourier transforms and their interpretation in a mini-MATLAB project. This section is generally the most challenging for students.

Part 4 returns to material that is usually covered in a standard course on multivariate calculus (third semester of a traditional calculus sequence). By this point in the course, students have become comfortable with working with expressions in multiple variables. Visualization in three dimensions is taught, as well as partial derivatives and multiple integrals. There is an emphasis on physical interpretation of these quantities. However, the level of coverage is not as extensive as a typical third semester calculus course. For example, a topic from a typical course in multivariable calculus that is not covered in MfC is Stoke's Theorem.

The concluding part, the shorter Part 5 is a basic introduction to partial differential equations. Students are introduced to separation of variables and the method is applied to solve the heat equation and the classical wave equations. Boundary conditions and initial conditions are discussed, again with an emphasis on modeling a physical system. This is a topic that students would not encounter until a course in partial differential equations after a course in ordinary differential equations, a course that very few chemistry students take. We considered taking more time in Part IV and omitting Part V, but an advantage of covering Part V is that many concepts from the course come together when solving partial differential equations. Indeed, this topic allows students to combine their knowledge of ordinary differential equation boundary value problems, partial derivatives, and Fourier series. Another advantage is that students are likely to see the wave equation near the start of a physical chemistry course, and we want them to feel like they are mathematically prepared from the beginning of the course.

Near the end of MfC, students are assigned a group project, applying separation of variables. This project is discussed further in Section 4.

To allow for this material to be covered in a year-long course, some sacrifices from the traditional sequence clearly need to be made. This includes some integration techniques and theorems on convergence of sequences and series as well as Stoke's theorem. Although the topics covered in MfC range from differential equations to linear algebra to understanding multivariable relationships, the fact that they are tied together by a theme of linear operators helps to unite the course and allows for the reinforcement of previously learned topics throughout.

The focus of this course is on developing students' mathematical dexterity and reasoning skills with motivation coming from chemistry. One challenge is that some of the most compelling examples require a good deal of chemistry to understand. For example, students were assigned a project on Nuclear Magnetic Resonance (NMR). This is a compelling application of Fourier transforms. However, the theory on molecular structure and NMR is taught in Organic chemistry. The students who had taken organic chemistry (*i.e.* had seen NMR in a classroom setting) thought the application was neat, though oversimplified. The students who had not had an organic chemistry course, could perform the transform but were at a loss when it came to connecting the output signal to the molecular structure, even with an (oversimplified) explanation in the project description.

At the end of the second semester, students were given a final group project. Students are guided through the analytic solution to the Schrödinger equation for the hydrogen atom. This project pulls together concepts from operators, correct handling of multiple variables, partial derivatives, techniques of solving differential equations and partial differential equations, visualizing in three dimensions, and the postulates of quantum mechanics in an example that is very compelling for chemistry students.

Impact in Physical Chemistry Course

The difference in students completing the calculus sequence versus the MfC sequence to fulfill their mathematics requirements for chemistry is dramatic. The difference in students’ daily engagement in the Physical Chemistry course is different between the two student populations. For example, in Physical Chemistry 1, students that have taken the MfC course sequence have already been exposed to the concept of a differential equation so they do not have to grasp what a differential equation is before striving to understand the interpretation of the solutions they generate for the Schrödinger equation. Instead, students that have taken the MfC sequence are confident in their practical knowledge of finding solutions to ordinary differential equations. Thus, they have the capacity and are free to begin thinking about the interpretation of solutions to the Schrödinger equation, rather than being stuck on mathematical mechanics associated with solving differential equations. Likewise, students having completed MfC approach the Maxwell relations in thermodynamics without trepidation having already manipulated partial differential equations. These are only two of many examples that speak to the divide that MfC bridges by producing a course that nests the mathematics required as a chemistry practitioner in chemical applications.

The feedback from students who have taken MfC and then physical chemistry has been positive. These students have encouraged their colleagues to take MfC rather than the traditional Calculus sequence, noting that students having taken the traditional Calculus sequence struggle more in Physical Chemistry than students having taken the MfC course sequence. Even students who struggled in MfC have remarked how familiar they found the math in physical chemistry, which improved their outlook about the traditionally dreaded physical chemistry course.

Finally, MfC offered at CSU does not require additional credit hours of math for our chemistry majors. Instead, we have tailored the mathematics and the application of the mathematics to be aligned with the needs of a chemistry practitioner. To accommodate transfer students and students changing majors, we still allow chemistry majors to take the traditional three semesters of Calculus for Physical Scientists, but strongly urge our majors to take MfC.

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