Chemistry

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Summary

Six themes for the mathematical preparation of students in the chemical sciences emerged from the chemistry workshop. These themes are (1) emphasizing multivariable relationships from the outset; (2) illustrating numerical methods applied to practical problems; (3) recognizing that chemists and biochemists depend heavily on visualizations, which are often three-dimensional; (4) paying attention to scale, units and estimation; (5) knowing that skill in mathematical reasoning is widely applicable; and (6) including practice in analyzing large data sets. Theme 5 is an especially important contribution. The mathematicians play an essential role in helping chemistry students learn how to think in logical and formal ways that are essential in the chemical sciences. Chemistry students also must learn how "to listen to the equations."

The teaching of mathematical methods for chemistry is a responsibility shared by chemists and mathematicians. The role of chemists in teaching mathematical methods increases with the level of the course work in most areas of chemistry. To be concrete about this sharing of responsibility between chemists and mathematicians, the members of the workshop developed an explicit classification presented in tabular form. Four categories for the teaching of mathematics are distinguished. They are (1) mathematical material learned in secondary school, which chemists reinforce; (2) mathematical material chemists expect mathematicians to develop; (3) mathematical material for which chemists have responsibility at the general chemistry level; and (4) mathematical material for which the chemists have responsibility in advanced courses.

No pattern in the use of powerful software tools for mathematics exists in chemistry instruction at present. Chemists use *Mathematica*, *Matlab*, and *Mathcad* to variable extents. Thus, chemists do not recommend standardizing on one of these. However, chemists make extensive use of spreadsheets. More use of spreadsheets in calculus courses would anticipate their use in chemistry. In addition, chemists are more dependent on computers than on graphing calculators.

Chemists are as concerned about the writing skills of students as are the mathematicians. Thus, chemists welcome the new emphasis on having students in mathematics express concepts in clear writing as well as symbolically. For instruction in mathematics to have greater relevance to other disciplines, problems are needed that are of disciplinary significance but expressed in terms understandable to mathematicians and their students. Chemists recommend that mathematicians actively solicit such problems and make them widely available.

Narrative

Introduction and Background

Mathematics in the Chemistry Curriculum. The range of mathematics needed for chemistry is enormous. The range extends from the relatively modest levels used by synthetic organic chemists through greater use by inorganic chemists and biochemists to extensive use by physical chemists, computational chemists and theoretical chemists. For theoretical and computational chemists the level and uses of mathematics are without limit. For analytical chemists, statistics is much more important than in other areas of chemistry. For all of the subfields within chemistry there is dependence on thinking quantitatively and on using spatial models of molecular systems. All chemists agree that undergraduates should have a good foundation in mathematics.

All chemistry and biochemistry students and students in other variations on the chemistry major take at least two semesters of calculus. Often, three semesters of mathematics are required for the B.S. major. In addition, many of the B.S. students take a semester of linear algebra or differential equations. In designing the mathematics curriculum, it is important to recognize that the first two semesters of calculus are common to all versions of chemistry majors.

It is exceptional for chemistry students to take a course in statistics in a mathematics department. Nonetheless, considerable instruction in statistics and use of statistical inference occurs in analytical chemistry courses and to a lesser extent in physical chemistry courses.

Lower-division courses, including first-year courses and organic chemistry courses, serve a wide range of students in various majors in the sciences, including biology, neuroscience, earth sciences and engineering. Few students take these courses as part of a broad education, although some students do so before switching to a major outside the sciences. Of the students who take courses in general chemistry, a large fraction intend to major in the biological sciences or to complete the requirements for medical school. Another substantial fraction in many universities and at some colleges are in engineering.

For the first-year courses, chemists do not assume that all students have taken or are taking calculus, although special sections are often taught for the mathematically inclined. Those students who will major in chemistry and biochemistry are a modest fraction (5–10%) of the students enrolled in first-year chemistry and organic chemistry. Despite the range of the audience for lower-division courses, it is appropriate to regard all these students as interested in growing in scientific and mathematical proficiency. For the purpose of the workshop, however, the chemistry group followed the charge presented and focused on the preparation of chemistry and biochemistry majors.

Several challenges in teaching chemistry are related to mathematical usage. One such problem is making connections between the real world of tangible chemical material and the abstractions that are used to understand these materials and their transformations. An important aspect of these abstractions lies in relating the microscopic (nanoscale) world of molecules to the macroscopic world of real chemical material. The models that describe the nanoscale world are often mathematical, and the bridges between the nanoscale world and the macroscopic world are generally crossed with mathematical reasoning. The mathematical description of chemical material is typically multivariate, a reality that does not correlate well with the emphasis on single variable functions in the typical first two semesters of instruction in calculus. In addition, chemistry students would be better prepared if they encountered a variety of variables other than the standard x, y, z set.

Chemists are aware of the calculus reform movement, but they are generally unaware of its outcomes. At the opening session of the workshop David Bressoud provided a helpful summary of the principal outcomes of calculus reform.

Perspectives of the Workshop. The group of chemists assembled for the workshop at Macalester College was weighted toward physical chemists. In addition, some were analytical or inorganic chemists by training. No organic chemists or biochemists were in the group. Two of the participants (Craig and Engstrom) were members of the Committee on Professional Training (CPT) of the American Chemical Society (ACS). They were charged with linking the deliberations in the Mathematics Workshop to the work of the CPT, which develops guidelines for undergraduate curricula in chemistry and its subfields and reviews compliance of chemistry departments with these guidelines.

The chemistry group focused on questions in the Understanding and Content cluster and in the Technology cluster of the instructions from the MAA. The chemists had some difficulty in making a sharp distinction between conceptual principles and problem-solving skills, which were distinguished under the heading of Understanding and Content. That blurring is evident in some of the specific recommendations from the chemistry study group.

Six Themes. Six themes for the mathematical preparation of chemistry students emerged from the extensive discussion of the first two clusters of questions. Mathematicians are asked to keep these six themes in mind as courses in mathematics are redesigned. Reinforcement in mathematics courses of student learning in the areas of the six themes makes the teaching of chemistry more effective. A consideration of each of the six themes follows.

1. *Multivariable Relationships*. Almost all problems in chemistry from the lowly ideal gas law to the most sophisticated applications of quantum mechanics and statistical mechanics are multivariate. Thus, it is desirable that calculus courses address multivariable problems from the outset.
2. *Numerical methods.* Numerical methods are used in a host of practical calculations in chemistry, most enabled by the use of computers.
3. *Visualization*. Chemistry is highly visual. Synthetic chemistry, which involves understanding the properties and transformations of small and large molecular assemblies, depends on practitioners being able to visualize structures and atomic and molecular orbitals in three dimensions. Understanding the consequences of quantum mechanics for chemical bonding and appreciating graphical representations, often multidimensional, depend on sophisticated visualizations.
4. *Scale and estimation*. The stretch from the nanoscale world of atoms and molecules to tangible material is of the order of Avogadro's number, which is about 10^{24}. Microscale chemistry is 10^6 or so smaller than tangible size (micrograms versus grams). Laser pulses that interrogate intimate changes in molecular species during chemical reactions may be only 10^{-15} s in duration. Other processes of interest occur on time scales up to the age of the earth (10^{17} s). Thus, distinctions in scale, along with an intuitive feeling for the different values along the scales of size, are of central importance in chemistry. Back-of-the-envelope calculations done to order-of-magnitude accuracy are sufficient in some cases and essential for checking the reasonableness of more detailed calculations. The careful use of units is an aid to approximations as well as to exact calculations.
5. *Mathematical reasoning*. Facility at mathematical reasoning permeates most of chemistry. Students must be able to follow and apply algebraic arguments, that is, "listen to the equations," if they are to understand the relationships between various mathematical expressions, to adapt these expressions to particular applications, and to see that most specific mathematical expressions can be recovered from a few fundamental relationships in a few steps. Logical, organized thinking and abstract reasoning are skills developed in mathematics courses that are essential for chemistry. At the physical chemistry level students must be able to follow logical reasoning and proofs, which is enabled by previous experience in mathematics courses. Careful use of notation also needs to be reinforced.
6. *Data analysis*. Data analysis is a widespread activity in chemistry that depends on the application of mathematical methods. These methods include statistics and curve fitting.

Answers to the Mathematicians' Questions. Because the principal goal of the workshop was to provide advice for the planning and teaching of the mathematics curriculum, providing a full account of the role of mathematics in the teaching of chemistry might be regarded as unnecessary. It seemed to the chemists, however, that attempting to isolate the part of instruction in mathematics for which the mathematicians alone have principal responsibility would be misleading. The importance and scope of mathematics in chemistry would not be fully apparent. Opportunities for linkages between chemistry and mathematics would be lost. Furthermore, chemists are unaccustomed to isolating their use and teaching of mathematics from what students have learned from mathematicians. Thus, the chemists provided a comprehensive survey of the role of mathematics in chemistry and of how instruction in mathematics should be delivered as part of the whole.

In discussions with the mathematicians the chemists confirmed their suspicion that geometry has been largely squeezed out of the secondary school curriculum. Little background in geometry helps explain why chemistry students have growing difficulty with the spatial relationships that are at the heart of much chemical thinking. The disappearance of plane geometry also removes a significant early exposure to formal proofs.

Understanding and Content

In their discussion of concepts and skills, the chemists identified several categories for specifying the locus of responsibility for instruction in mathematics. Specific conceptual principles are listed in the table in Appendix A, and specific skill areas are listed in the table in Apendix B.

The first category, designated **1** in the tables in the appendices, is conceptual material or skills that chemists expect students to bring to the first-year chemistry course from their preparation in secondary school. Chemists recognize that students will have to be reminded of many of these concepts or skills and have them reinforced and extended in the context of the chemistry course. Such teaching is the responsibility of the chemistry faculty.

The second category, designated **2** in the appendices, is conceptual material and skills that chemists expect the mathematics faculty to develop.

The third category, designated **3**, is conceptual material and skills in mathematics for which the chemists have principal responsibility. Some of this material is of a more general nature and would be developed in the lower division courses at the same time students are learning calculus. This type of instruction is designated **3G** in the appendices, where **G** stands for general. Other material is of an advanced nature and would be developed in advanced chemistry courses after students have taken the expected mathematics sequence in college. In the appendices, this type of instruction is designated **3A** , where **A** stands for advanced. Such teaching of mathematical concepts in the context of chemistry is especially effective. Revisiting mathematical methods and seeing them applied in a different context also reinforces learning.

In the classification scheme in Appendix A and Appendix B, just described, it is category **2** that is of direct importance to the mathematicians as they plan their courses. Recognizing that the list of desirable concepts for mathematics instruction is long, the concepts are prioritized in two groups. Those that are given the highest priority are in **boldface type**. The others are of second priority.

In the summing-up session with biologists, chemists and mathematicians present, the chemists were asked how the use of mathematics relates to the typical education in chemistry for students in the biological sciences. The classification scheme in the appendices provides a direct answer. The experience for students in the biological sciences consists of categories **1** and **3G**.

Technology

Technology makes it possible to address old questions more quantitatively and more realistically than was possible in the past. The complexities of real chemical material can be approached more fully. Examples of old questions are chemical equilibrium, chemical bonding, reaction mechanisms, and interpretation of spectral data. In general, solving these problems depends on multivariate analysis and numerical methods. Use of computers is assumed.

The usefulness of graphing calculators does not rank high with chemists. Chemists worry that the indiscriminate use of graphing calculators in high school mathematics may interfere with students' learning the basic concepts. Graphing calculators do provide an effective means of exploring quantitative relationships once students have mastered the fundamentals of those relationships. Chemists use the software tools *Mathematica*, *Matlab*, or *Mathcad*; *Mathcad* is the most popular. However, no pattern in the use of these materials in chemistry justifies a recommendation about standardizing use in mathematics courses. Of widespread use in chemistry teaching and research are spreadsheets, including the graphing and statistical analysis features. Spreadsheets can be used to show graphically how functions respond to changes in parameters and to show how approximations evolve. Chemists would welcome the use of spreadsheets to teach calculus. Chemists are more likely to use computers than calculators for most applications.

Uses of Technology

1. Multivariate modeling and visualization.
2. Iterative solutions.
3. Access to and use of databases such as those of the Cambridge Crystallographic Data Centre, National Institute of Standards and Technology files for smaller molecules, Beilstein, Chemical Abstracts Services, and the Protein Data Bank.
4. Data collection—high speed and extensive.
5. Data analysis such as in Fourier transform nuclear magnetic resonance and most other forms of modern spectroscopy.
6. Experimental design.
7. Pattern recognition.
8. Combinatorial chemistry in which numerous variations on a chemical reaction are run in parallel and then the efficacy of the various products is tested. Such methods are now widely applied for drug discovery, for developing new light emitting diodes and the like. Robotics and computer handling of the plethora of data are essential features of such work.
9. Facilitating interdisciplinary investigations. Internet collaborations.

Instructional Techniques

Today's mathematicians and chemists agree on the value of having students write to learn mathematics and chemistry. A laudable goal of the calculus reform movement is to have students write to foster critical thinking skills. Chemistry students, in particular, need to be confident about mathematics as an active language. Chemists have become more systematic in having their students write significant reports and critiquing these reports in supportive ways. The chemists applaud similar efforts within the mathematics community.

Instructional Interconnections

The chemists agreed that communication has been inadequate between mathematicians and chemists regarding the curriculum of mutual interest. They applauded working toward reform in communication between the disciplines as well as reform within the disciplines.

A concrete proposal for strengthening the linkage between mathematicians and chemists is to have chemists provide a set of representative problems in which various mathematical methods are crucial. These chemical problems would be expressed in language understandable to mathematicians. These problems should also be ones that could be used to teach students in mathematics courses. The initiative for starting such a process lies with the mathematicians.

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APPENDIX A. Understanding and Content, Conceptual Principles Classification Scheme

Who Teaches Material*

		1	2	3G	3A
1.	Basic mathematics. Algebra; scientific notation; graphing; ratios; percent; shapes, simple geometry, Platonic solids; solution to the quadratic equation; functions and their graphical expression: exponential, logarithmic (base *e* and base 10), polynomial, trigonometric; solving sets of equations.	X			
2.	Elementary statistics. Uncertainty in numbers representing experimental data, average, standard deviation.	X			X
3.	Units, conversion of units, scaling in powers of 10.	X			X
4.	**Calculus.** Differentiation, integration, limits, slopes, curvature, extrema, series, areas, volumes, graphical presentation of functions from $f(x)$ and from $f''(x)$. Multivariable. A standard set of derivatives and integrals related to functions listed in 1 should be memorized. Inverse relationships. Varying the symbols used for variables. Integration by parts. Exact and inexact differentials; Euler reciprocity relationship for exactness of differentials. Careful specification of which variables are held constant in a partial derivative.		X		X
5.	**Creating, using, and interpreting graphs.**	X	X	X	X
6.	Estimating and making appropriate assumptions. Checking answers for reasonableness, relative importance of terms in equations, appropriate use of linear approximations and Taylor series.	X	X	X	X
7.	Iteration. The Newton methods, gradients, iteration consisting of initialization, successive approximation, and termination steps.		X	X	X
8.	Coordinate systems (Cartesian and polar) and transformations between them. Different frames of reference for coordinate systems.		X		X
9.	Numerical methods. For integration, differentiation, differential equations, finding roots.		X		X
10.	Representation of information. Digital-to-analog and analog-to-digital conversions. Consequences of using different number bases or fractional expressions. Binary, octal, hexadecimal. Enhancement in signal/noise ratio from multiple scanning in which the signal increases linearly with the number of scans, whereas the noise, which is statistical, increases by the square root of the number of scans.		X		X
11.	Statistics. Probability, combinatorics, distributions, uncertainty, confidence intervals, propagation of error.		X		X
12.	Curve fitting. Least-squares methods, regression, using different weights for data, deconvolution (separating out the contributions of several curves of assumed functionality from their overlap in a complicated curve).		X		X
13.	Operators. How they combine and interact. Precedence.		X		X
14.	**Spatial representations.** 3-D geometry, surfaces, projections, slices, perspective.	X	X	X	X

Who Teaches Material*

		1	**2**	**3G**	**3A**
15.	Group theory.				X
16.	**Linear algebra.** Matrix algebra, eigen analysis, basis functions, orthogonality, Fourier series.		X		X
17.	Differential equations. First-order DEs. First-order separable. Partial DEs.		X		X
18.	Symmetry. Transformations. Operators. Symmetric and antisymmetric functions.		X		X
19.	Chemometrics. In its broadest sense chemometrics is the use of mathematical techniques and computational methods to assist the chemical scientist in making and interpreting chemical measurements. Chemometrics includes univariate statistics, multivariate statistics, multivariate modeling (e.g., least-squares regression, partial-least-squares regression), convolution and correlation, pattern recognition, Fourier methods, the calculus, optimization methods (e.g., simplex), and experimental design. The emphasis in recent years has been on extracting useful qualitative and quantitative information from large sets of multivariate data and in developing mathematical models that can predict chemical properties from chemical structure.				X

***1** Material learned in secondary school, which chemists reinforce.

2 Material chemists expect mathematicians to develop.

3G Material in mathematics for which chemists have responsibility at the general chemistry level.

3A Material in mathematics for which chemists have responsibility at the advanced course level.

Concepts with the highest priority are indicated by **boldface.**

APPENDIX B. Understanding and Content, Skills Classification Scheme

Who Teaches Material*

		1	2	3G	3A
1.	Spreedsheets.		X	X	
2.	Graphing.	X	X	X	
3.	Computer algebra (symbolic mathematics by computer).		X		X
4.	Numerical algorithms, iteration.		X		X
5.	Modeling. Analytical (interacting functions such as in a multistep rate process) and molecular (exploring molecular structure and wave functions).			X	X
6.	Graphics software and other visualizations.				X
7.	Algorithms. Understand and apply them (e.g., in Excel and Matlab).		X		X
8.	Reading mathematical expressions and writing them with understanding.	X	X	X	

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