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 math-
ematics 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 chem-
istry 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 engi-
neering. 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 under-
stand 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 mod-
els 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 sin-
gle variable functions in the typical first two semesters of instruction in calculus. In addition, chemistry stu-
dents 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 out-
comes 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 train-
ing. 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 prop-
erties 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 con-
sequences 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 mate-
rial is of the order of Avogadro’s number, which is about 10^{24}. Microscale chemistry is 10^6 or so small-
er 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 inter-
est 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 mathemat-
ics 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 Appendix 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.
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.

**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.
WORKSHOP PARTICIPANTS

Mathematics Participants

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William F. Coleman, Physical/Inorganic Chemistry, Wellesley College
Royce C. Engstrom, Analytical Chemistry, University of South Dakota
Peter C. Jurs, Analytical/Computational Chemistry, Pennsylvania State University
Joseph J. Lagowski, Inorganic Chemistry, University of Texas Austin
A. Truman Schwartz, Physical Chemistry, Macalester College
Theresa Julia Zielinski, Physical Chemistry, Monmouth University

Mathematics Participants

David Bressoud, Mathematics, Macalester College
Thomas Halverson, Mathematics, Macalester College
Roger Howe, Mathematics, Yale University

ACKNOWLEDGEMENTS

The participants in the chemistry workshop thank Macalester College for the fine arrangements and the warm welcome we enjoyed during our work on this project. David Bressoud played a crucial role in setting up the workshop, a gathering that provided opportunities for chemists and biologists to discuss the important matter of undergraduate instruction in mathematics with mathematicians. We also thank the CUPM of the MAA for having the wisdom to consult with faculty members in other disciplines whose students depend on instruction in mathematics. We are grateful for support of the workshop at Macalester College by a grant from the NSF, by an institutional grant from the Howard Hughes Foundation, and by Macalester College.
# APPENDIX A. Understanding and Content, Conceptual Principles Classification Scheme

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3G</th>
<th>3A</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>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.</td>
<td>X</td>
<td></td>
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<tr>
<td>2.</td>
<td>Elementary statistics. Uncertainty in numbers representing experimental data, average, standard deviation.</td>
<td>X</td>
<td>X</td>
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<tr>
<td>3.</td>
<td>Units, conversion of units, scaling in powers of 10.</td>
<td>X</td>
<td>X</td>
<td></td>
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<tr>
<td>4.</td>
<td><strong>Calculus.</strong> 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.</td>
<td>X</td>
<td>X</td>
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<tr>
<td>5.</td>
<td><strong>Creating, using, and interpreting graphs.</strong></td>
<td>X</td>
<td>X</td>
<td>X</td>
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<tr>
<td>7.</td>
<td>Iteration. The Newton methods, gradients, iteration consisting of initialization, successive approximation, and termination steps.</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<tr>
<td>8.</td>
<td>Coordinate systems (Cartesian and polar) and transformations between them. Different frames of reference for coordinate systems.</td>
<td>X</td>
<td>X</td>
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<tr>
<td>10.</td>
<td>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.</td>
<td>X</td>
<td>X</td>
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<tr>
<td>12.</td>
<td>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).</td>
<td>X</td>
<td>X</td>
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<tr>
<td>14.</td>
<td><strong>Spatial representations.</strong> 3-D geometry, surfaces, projections, slices, perspective.</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td></td>
<td>Who Teaches Material*</td>
<td></td>
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<tr>
<td>15</td>
<td>Group theory.</td>
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<tr>
<td>16</td>
<td><strong>Linear algebra.</strong></td>
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<tr>
<td></td>
<td>Matrix algebra, eigen analysis, basis functions, orthogonality, Fourier series.</td>
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<tr>
<td>19</td>
<td>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.</td>
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</tbody>
</table>

*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

<table>
<thead>
<tr>
<th>Who Teaches Material*</th>
<th>1</th>
<th>2</th>
<th>3G</th>
<th>3A</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Spreadsheets.</td>
<td></td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>2. Graphing.</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
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<tr>
<td>3. Computer algebra (symbolic mathematics by computer).</td>
<td></td>
<td>X</td>
<td>X</td>
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<tr>
<td>4. Numerical algorithms, iteration.</td>
<td>X</td>
<td>X</td>
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<tr>
<td>5. Modeling. Analytical (interacting functions such as in a multistep rate process) and molecular (exploring molecular structure and wave functions).</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7. Algorithms. Understand and apply them (e.g., in Excel and Matlab).</td>
<td>X</td>
<td>X</td>
<td></td>
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</tr>
<tr>
<td>8. Reading mathematical expressions and writing them with understanding.</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
</tbody>
</table>

*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.

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