Engineering: Chemical Engineering

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Summary

It is clear that application of mathematical concepts and the generation of mathematical solutions to engineering problems are essential to the educational programs of all undergraduate engineering students. Enhanced cooperation between the mathematics faculty and the engineering faculty can lead to a better experience for our students.

Without exception, this group felt that the workshop was a very productive way to promote dialogue between the mathematics and engineering education communities and we would like to see workshops of this type continue to be held. Another venue that mathematics educators may want to explore is the American Society for Engineering Education (www.asee.org), which has a mathematics division. On the other hand, it may be productive for engineering educators to attend MAA meetings. Perhaps most importantly, mechanisms need to be implemented to promote interaction between engineering and mathematics faculty within individual universities — good relationships at this level will enable mathematics faculty to understand what material the engineering faculty would like to see reinforced and emphasized, as well as enabling engineering faculty to gain a better understanding of the issues surrounding mathematical preparation of entering freshman engineering majors.

Narrative

Introduction and Background

What are Chemical Engineers? Since this is a report for mathematicians, we thought an appropriate introduction would be to try to say what chemical engineers do, why we need mathematics, and how we use it. A reasonably broad definition of what we do is that chemical engineers design materials and the processes by which materials are made. Traditionally, chemical engineers have been associated with the petroleum and large-scale chemical industries, but especially in recent years, chemical engineers have been involved in pharmaceuticals, foods, polymers and materials, microelectronics and biotechnology. The core subjects that underlie and unify this broad field are thermodynamics, chemical reaction processes, transport processes (i.e., the spatial and temporal distribution of mass, momentum and energy) and process dynamics, design and control.

On top of this fundamental framework, a central emphasis of chemical engineering education is model building and analysis. A good chemical engineer brings together the fundamentals to build and refine a mathematical model of a process that will help him or her understand and optimize its performance. To be

good at model building and analysis, students must have at hand the mathematical background to understand and work with the core scientific areas, as well as to find solutions to the final model that they build. In this context, the "solution" to a mathematics problem is often in the understanding of the behavior of the process described by the mathematics, rather than the specific closed form (or numerical) result.

Here's an example. A starting point for understanding any process is writing down the conservation laws that the system or process satisfies: for conserved quantities, accumulation = input – output. Depending on the level of detail of the model, this equation might be, for example, a large set of linear algebraic equations that determine the relationships between fluxes of chemical species throughout the process (a species balance), or it might be a set of parabolic partial differential equations governing the temperature and composition of the fluid in a chemical reactor. In the thermodynamics of multiphase systems, energy is conserved but takes on a variety of forms; a good knowledge of multivariable differential calculus is essential here to keep track of everything.

Understanding and Content

Mathematics for Chemical Engineering. We do not view our role here as one of prescribing the mathematics curriculum—we do not want mathematics instruction to provide only what students can "get by" with knowing. Nor do we want to come down on either side of the "traditional" vs. "reform" debate—it is likely that both sides are right, to an extent. We have collected here some general thoughts on subject matter and emphasis that arose in our discussions:

Precalculus Foundations. By foundations, we mean

- basic knowledge of families of functions (polynomial, exponential...) in terms of data, graphs, words and equations, basic trig identities, properties of logarithms,
- equations, inequalities,
- basic logic and algorithms,
- small linear systems of equations,
- · coordinate systems,
- basic arithmetic and manipulation skills.

Mastery of the above areas is crucial. Probably the most important thing the mathematics education community can do here is to actively critique the pedagogy of K-12 education—to help sort out which "reforms" are productive from those that are merely ed-school fads and to encourage schools not to neglect the education of the more mathematically inclined students by focusing the curriculum too narrowly on the average performer. Another important role here is to provide programs that help K-12 mathematics teachers understand something about the applications of the mathematics that they teach (engineering faculty should do much more here).

Linear Mathematics. We feel that our students would benefit from earlier exposure to the basics of linear systems in \mathbb{R}^n , particularly

- the geometry of linear spaces,
- vector algebra (especially in 3D),
- **Ax** = **b** (existence and uniqueness, Gaussian elimination, geometric interpretation, over- and under-determined systems and least squares problems),
- Ax = lx (characteristic polynomial and diagonalization, Jordan form, range and nullspace of A, geometry).

At Wisconsin, there is a course on "linear mathematics", which introduces these notions and applies them to systems of ordinary differential equations (see below). Many chemical engineering students take this in lieu of the traditional differential equations class.

Calculus and Differential Equations. In our discussions of calculus, the importance of visualization repeatedly arose, especially as a guide to differential and vector calculus in multiple dimensions, plotting (e.g., what function is linear on a log-log plot?), working in cylindrical and spherical coordinate systems and how to convert between coordinate systems. Though students must learn techniques such as integration by parts, somewhat less time could be spent on techniques for evaluating complicated integrals. The time saved could be spent on topics such as visualizing the application of the chain rule in multiple dimensions. Understanding of truncated Taylor series for local approximation of functions is very important and should be seen early and often. In differential equations, a thorough knowledge of linear constant coefficient systems (IVPs and BVPs; see above) is preferable to emphasis on existence theory and series solutions for non-constant coefficient problems. Some qualitative theory for nonlinear systems would be nice.

Probability and Statistics. Alumni surveys typically show that probability and statistics, in addition to the extensive use of spread-sheeting software, is the most common application of mathematics for the practicing chemical engineer with a Bachelor of Science degree. Key issues here include parameter estimation, experimental design, sampling and the origins and properties of various distribution functions.

Students interested in graduate school should be encouraged by their mathematics professors as well as their engineering advisors to take additional mathematics courses. A final general comment: for engineers, concepts are more important than proofs, but students should have some idea of the power of a theorem. In other words, we are comfortable with students learning mathematical facts without necessarily having seen the proof.

Technology and Instructional Techniques

A fair amount of the discussion at the workshop, within our group and others, centered around the use of "technology" in the mathematics courses for engineers. In the discussions, "technology" meant a number of different things, from numerical methods to graphing calculators to symbolic manipulation packages. We'd like to emphasize here some points to be kept in mind when thinking of the introduction of these tools into mathematics courses. So here are two simple but common questions and our responses:

"Why should I learn to do it by hand?"

- sense of form of mathematical expressions, understanding of what manipulations are available, facility with these manipulations
- fluency in the language of mathematical concepts,
- appreciation and recognition of mathematical rigor,
- discipline, maturity, confidence of mastery,
- closed form results are best, if available,
- recognition of limitations of closed form results, where things get difficult,
- knowledge of what computers do

"Use of computers dumbs down the mathematics course—why use them?"

- solution of realistic (complex) problems, many of which involve numerical solutions—In upper level courses, extensive use is made of programs like *MATLAB*TM, *MathCad*TM, *Mathematica*TM, *Polymath*TM, and *Octave*. (GNU *Octave* is freely available at www.che.wisc.edu/octave.)
- efficient exploration of solution and design space
- visualization, especially in multidimensional and vector calculus
- relief from tedium
- · confidence in results derived by hand

Ultimately, we feel that the technology should take a back seat in mathematics courses until it becomes necessary to solve interesting problems. For example, in a linear algebra course, students should be able to do LU decomposition of a 3×3 system by hand before they are shown that *MATLAB* does it in one command. At the same time, it is useful to point out the relationship between numerical techniques and exact ones (e.g., a Riemann sum can be evaluated numerically to approximate an integral). Students should have a solid understanding regarding limitations of numerical methods and their accuracy. They should clearly see the power of analytical solutions when such solutions can be found.

Instructional Interconnections

A suggestion for coupling mathematics and engineering education. One set of issues that arose repeatedly in the workshop discussions was the concern that students don't see connections between mathematical tools, concepts and principles and their wide utility in engineering. A related concern was the time lag between exposure to mathematics and its application and importance in the solution of real engineering problems. The notion of "just-in-time" learning arose repeatedly, and the suggestion was made that the mathematics courses be more application- or example-driven and be more evenly spread through the curriculum, rather than "front loaded" into the first two years. Our group shares these concerns, but also feels that:

- (1) part of the beauty and power of mathematics is that it is example-independent—calculus applies to economics just as it does to mechanics,
- (2) the time spent developing the background for engineering applications is time not spent on mathematical principles and tools, and
- (3) a straightforward "just-in-time" approach will not satisfy all the engineering majors—electrical engineers do not need Laplace transforms at the same time as chemical engineers.

We propose that an alternate structure be considered for addressing these concerns, which are essentially about how to connect mathematics and engineering in the students' minds. We suggest the introduction of **discipline specific supplements**, especially for the calculus sequence. These could be workbooks or web pages, for example containing

- engineering background material, e.g., some basic thermodynamics, and how specific mathematical
 principles and/or tools (e.g., total differentials, partial derivatives in several dimensions) can be
 applied,
- exercises or projects integrating mathematics and engineering,
- additional discipline-specific emphasis, e.g. trigonometric identities and manipulations for electrical engineering students.

These could be used independently by the students, or used in a one-credit course running in parallel with the calculus courses, or simply be resources for mathematics instructors wishing to gain perspective on engineering applications or bring engineering applications into the mathematics classroom. This is perhaps overly ambitious, but we believe it is worth considering. Within chemical engineering, there is an organization called CACHE (Computer Aids for Chemical Engineering—www.CACHE.org) that may take a role in studying this possibility. Michael B. Cutlip of this working group will transmit this opportunity to the CACHE organization for possible coordination with the MAA.

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