CHEMISTRY AND LIFE SCIENCES IN A NEW VISION OF CHEMICAL ENGINEERING

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Chemical engineering must expand its self-concept in order to maintain its vitality and viability as a profession. It can still be defined as "the profession that applies chemistry." However, current chemical engineering education, however, does not effectively couple chemistry to engineering applications. This article proposes that the central issue of this profession's future is how to reintegrate chemistry, including life sciences, into our vision of chemical engineering. It is a challenge to be met in educational curricula, in practice, and within the restructuring of the chemical process industries.

Applying chemistry now must be understood to include applying the chemistry of life sciences. Chemical engineering's foundation in chemistry has been a solid basis for dominating the interface between process technology and the chemical sciences. The profession's relationship to life sciences has been hazier, deriving naturally—but often empirically—from parallels of bioreactors and bioseparations to traditional reactor engineering and separations. Much of the traditional profession still sees biochemical engineering as peripheral, and the lack of life sciences in the ChE curriculum shows how strong that perception is. Now, as biology is becoming chemically based, haziness should be cleared up.

Going still further, modern chemistry and biology have become more focused on understanding and exploiting the molecular scale, and so must chemical engineering. Reactions and physical properties alike have their bases in chemical structure. Chemical engineers should be at the forefront of translating this understanding into processes and products. Extra science courses aren't sufficient, as the disconnects between chemistry courses and chemical engineering courses show. Rather, the science and applications must be layered and mixed through the curriculum.

Molecularly based modeling is one aspect of these connections that chemical engineers will increasingly need to know. Over time, it must be added into the curriculum as a topic in its own right and as an educational aid to the larger goal of integrating chemistry. Use of this set of tools is penetrating the research activities of many companies, but it is also beginning to be a practical means for resolving many questions about engineering properties. The Schrödinger equation and statistical mechanics form its scientific principles, and computational quantum chemistry, molecular simulations, and computer visualization form its toolbox. It is not a substitute for understanding the relevant chemistry, however. For such problems, computer programs still are faster than they are intelligent.

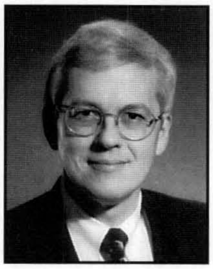
Applied chemistry—understood on the molecular and continuum scales, including biological chemistry, and tied more effectively into the profession and the rest of the ChE curriculum—must become a component of chemical engineering education that is equally important with transport phenomena, process operation and design, and economics. Chemical engineering faculties have a particular responsibility for reintegrating chemistry into chemical engineering because the undergraduate and graduate curricula reflect the profession's self-image to each new generation.

DEVELOPMENT OF CHEMICAL ENGINEERING'S PRESENT SELF-IMAGE

A profession's self-image is defined by

- *What its professionals do*
- *What they think others in their profession do*
- *What they are taught about the profession*

Consequently, it is useful to consider the undergraduate chemical engineering curriculum and how it has developed.



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The curriculum expresses what the faculty think the profession is or should be, and the courses of study also strongly influence the self-image of ChE students who go on to become its practicing professionals.

Historically, any ChE department's curriculum must be in accord with broad opinion, as articulated by the Accreditation Board for Engineering and Technology (ABET). Even though ABET now allows much greater latitude for departments to reshape their curricula, changes must be guided by careful study of feedback from their constituencies.

The key feature of chemical engineering practice is the economically feasible process. Realistically, *de novo* product invention has never been our calling card. It is natural, however, that product development will continue to be a collaboration between engineers and scientists, almost always linked by the requirement of a desirable product and the necessary process of making or formulating it. The link is only broken when the needed amount of product is tiny (scientists may carry out production) or when the science is already in place (product engineering).

Breadth is consequently another key aspect of chemical engineering's present self-image. Our profession is wonderfully inclusive, bringing together a wide range of sciences, technologies, and economics. It may not be quite true that "chemical engineers can do anything," as many have put it, but we do an amazing variety of things. The self-image of breadth in engineering education, coupled with particular depths, is somewhat deceptive. Historically, the education breadth has narrowed and become more specialized. Significantly, chemistry has always been at the heart of chemical engineering practice, but it has been pushed off to the edge of academic experience.

In the 19th century, the chemical engineer was a general engineer with a specialization in applied chemistry (Table 1). Courses involved much hands-on practical work, but most were usually "engineering" or "practical chemistry" or "industrial chemistry." The Civil War and the subsequent second industrial revolution had stimulated a burst of engineered production of oil products, of steel and smelted metals, and of manufactured tobacco products and refined sugar. The transportation industry (rail and ship) was a key factor to increased use and distribution of products, and demand for modern conveniences brought civic water and sewage systems, the coal-derived "gas-light" era, and dyed fabrics.

During the early 1900s, German chemists dominated industrial chemistry with their expertise in dyestuffs, coal conversion, and synthetic fertilizers. Petroleum refining in the U.S. focused on fuel uses. It was dominated by

TABLE 1

Examples of Curriculum Requirements for Chemical Engineers: 1898,[1] 1965, and 2000

Area	1898[1]	1965	2000
Chemical Engineering	Industrial Chemistry (including lectures and "laboratory for study of chemical processes on a larger scale")	Mass and Energy Balances Unit Operations (Heat Transfer and Fluid Flow) Equilibrium Separations Mass Transfer Operations Reactor Engineering Industrial Chemistry Process Design Process Control Unit Operations Laboratory	Mass and Energy Balances Transport Phenomena (Fluid Mechanics, Heat Transfer, Mass Transfer Operations) Equilibrium Separations Process Design Process Control Engineering Science and Process Laboratory
Other Engineering	Metallurgy and Forging Drafting Machining	FORTRAN Programming Engineering Graphics Statistics Intro. to Materials Intro. to Electrical Engineering	Communication and Computer Skills Engineering Science Electives
Mathematics		Calculus I, II, III Differential Equations	Calculus I, II, III Differential Equations
Chemistry (Some with Labs)	Gen., Org., Adv. Inorg., Theoretical, History of, and Sanitary Chemistry; Qual., Quant., and Gas Analysis	General Chemistry I and II Organic Chemistry I and II Physical Chemistry I (Thermodynamics and Kinetics)	General Chem. I and II Organic Chem. I and II Physical Chem. I (Thermody., Kinetics) II (Spectroscopy, Quantum Mech.)
Other Sciences (Some with Labs)	Mineralogy	Physics I and II Elective Intro. Course in Life Science	Physics I and II Elective intro. course in life science
Liberal Arts		English Composition Electives required in History, Economics	English Composition Electives required in Econ., Arts or Literature, History, Social Science

Rockefeller's Standard Oil trust until the 1911 court-mandated break-up and by its components afterward. World War I forced U.S. chemical companies to develop, such as Dow Chemical and Diamond Alkali (now part of Ultramar Diamond Shamrock).

The "Unit Operations" approach responded to these developments and the demand for quantitation in the early 20th century. Arthur D. Little and William H. Walker identified certain process elements as cutting across the variety of processes. Examples are fluid flow, heat transfer, distillation, and crystallization. Separation processes, based on equilibrium or on mass-transfer rates, were especially important. This approach provided a basis for moving from earlier batch and semibatch processing to high-capacity continuous processing. Textbooks by Walker, Lewis, and McAdams[2] pioneered the approach, and the text of McCabe and Smith[3] was a central text on the subject from the 1950s through the 1970s.

Transport Phenomena[4] still overshadows the chemistry of chemical engineering in U.S. curricula. No doubt, the intellectual appeal of its "clean" mathematics and physics is part of the explanation, contrasting sharply as it does with "messy" chemistry. "Clean" and "messy" are oversimplifications, but the dividing line between physics and chemistry has often been defined by the amount of mathematics and the degree of quantitation and precision. For example, compare mathematics in sophomore physics to the lack of it in sophomore organic chemistry. Motion of a pendulum may be treated rather exactly, but reactions of a Grignard reagent are organized by pattern recognition.

Physical chemistry is the point where students see mathematics and chemistry intersect. In their book, *Chemical Process Principles*, Hougen and Watson[5] chose to subdivide the physical chemistry of chemical engineering into mass and energy conservation balances, equilibrium thermodynamics, and kinetics. By comparison, modern physical chemistry courses have five main components: classical thermodynamics, kinetics, spectroscopy, quantum mechanics, and statistical mechanics.

Reactions have always been the most obvious part of chemistry in chemical engineering courses, appearing in courses on material and energy balances, thermodynamics, reaction engineering, and process design. Linkage to chemistry courses, however, is usually poor. Kinetics often appears only in the reaction engineering course, where reactor analysis is the emphasis and stoichiometric reactions are given to the student. Analysis is usually in terms of first-order reactions of "A goes to B." Inference of rates from ideal reactors gets good attention, and other power-law expressions are used to a small extent. Often, catalysis is not taught to undergraduates except via pseudo-homogeneous kinetics, although texts include heterogeneous treatments. Catalytic chemistry is treated as an empirical black box, and its chemical principles and classifications are seldom taught. Even at the graduate level, elegant treatments of reactor analysis and design (*e.g.* Aris' *Introduction to the Analysis of Chemical Reactors*[6]) have presumed that all of the needed chemical reactions, stoichiometries, and rate constants were known. Empirical kinetics and well-modeled reactors have served chemical engineers very well, but industrial practice has relied more and more on chemists to provide the reactions.

In the past, chemistry also appeared in "industrial chemistry" courses. These courses largely died out in the 1960s, strangled by their focus on flowsheet memorization rather than the chemical principles and components of the flowsheets. Also, as processes proliferated and became more confidential, flowsheets and details were less available for students, and these courses became less relevant.

At present (Table 1), the undergraduate curriculum typically includes a core of chemical engineering courses. It includes substantial formal study of mathematics, physics, and chemistry. Organic chemistry provides molecular structures and language for engineers to work with chemists, but its reaction chemistry seldom carries over to ChE courses. Physical chemistry emphasizes classical thermodynamics, which can be reinforcing or merely redundant when students often see two ChE thermodynamics courses as well. Spectroscopy may not be connected to practical chemical analysis. Elementary quantum mechanics may appear, but usually not statistical mechanics. Courses in life sciences are seldom required and are often limited to a freshman-level introductory course in biology, genetics, ecology, or medical issues.

CHEMICAL ENGINEERING IN EVOLVING PRACTICE

Meanwhile, the ChE professional has worked in a steady range of job types, but within dramatically changing industries. The process engineer has long typified the image of the chemical engineer, employing mass and energy balances, equilibrium and rate analyses, economics, and the engineering problem-solving skill of de-constructive analysis in order to operate and improve processes. Stereotypically, the process engineer would work in a large company. Many work instead in small companies as all-purpose chemical engineers.

There are many other roles as well. New engineers often move quickly into management roles, using different blends of many of the same talents, augmented by a greater role for communications and organizational skills. There are opportunities in product development, although chemists may dominate. Process design engineers, R&D engineers, and educators are other clearly visible career tracks for ChE students. When the economy is good, starting companies and consulting are easier than ever for students to imagine. Many chemical engineers are in sales and marketing.

As at the turn of the 20th century, the turn of the 21st century finds many chemical engineers working for oil and chemical companies. Continuous processes now dominate the plants, yet the spectrum of products is broader. Refineries produce a host of different fuels, byproducts, and chemicals that include elastomers, thermosets and thermoplastics, specialty chemicals, and fine chemicals.

In striking contrast to 1900, however, many chemical engineers are also working in food, personal care, materials, electronics, pharmaceuticals, and environmental-control industries. Figure 1 shows that these sectors employ approximately 33% of all chemical engineers working in industry and 38% of new chemical engineering graduates who took jobs in industry during the last three years. Chemical and fuel companies employed 41% of all chemical engineers and all new chemical engineering graduates. In contrast, in 1991 only 22% of chemical engineering graduates entered these newer sectors, while 63% went into chemical and fuel companies. The pie-chart in Figure 1 shows the electronics sector with a disproportionately larger portion of the employment of new graduates relative to all chemical engineers, while other sectors are quite comparable.

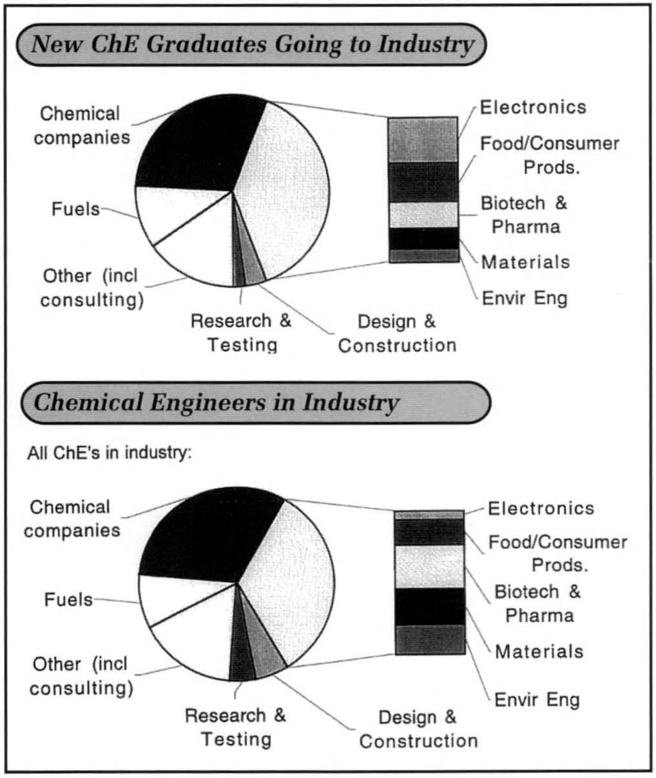

Figure 1. *Current distribution of industrial jobs in chemical engineering. TOP: New graduates going into industry, 1997-2000. Three-year average, weighted by number of BS (2,870 in survey, 52.3% going directly to industry), MS (520, 42.7%), and PhD graduates (380, 55.1%) in 2000 survey from 77 of 177 U.S. and Canadian chemical engineering programs.[7] Graduates not reported as going to industry are mostly continuing to academic institutions or do not report their employment. Total number of BS graduates is approximately 6,000 per year. BOTTOM: Full-time salaried chemical engineers in industry, interpreted from AIChE Career Services data.[8]*

Significantly, several chemical companies have begun adding more biologically oriented business. Part of the driving force behind this movement has been an optimistic belief in the lucrative nature of the pharmaceuticals business. Part is building on businesses in chemically synthesized agricultural products, and another part is the belief that bioprocessing and biomimetic processing can replace important nonbiological processes. Monsanto made a major commitment to applied life sciences, eventually splitting off its chemicals business as Solutia. DuPont, the oldest of the American chemical companies, joined with Merck to form a joint pharmaceuticals business, later buying out the venture as DuPont Pharmaceuticals. In June of 2001, however, it announced sale of this business to Bristol-Myers Squibb. Bayer has also built a strong life-sciences business and has chosen to keep it closely tied with its chemicals business.

LINKING CHEMISTRY AND BIOLOGY INTO CHE PRACTICE AND EDUCATION

These changed needs require a new vision of a more chemistry-centered chemical engineering. Process development and operation must be "faster, better, cheaper" (the pragmatist's mantra), requiring more effective understanding of the science and of how to apply chemical knowledge combined with physics and economics. "Product engineering" is yet another application of these combined principles. New understanding and tools of molecular-scale chemistry and molecular biology can help us achieve this vision.

This goal can be accomplished by

- *A better coupling of chemistry to solving engineering problems, using molecular perspectives as the basis for improvement*
- *Incorporating relevant life sciences (biochemistry, microbiology, and molecular biology) and their engineering applications using a molecular, chemical viewpoint*
- *Beginning to exploit computational quantum chemistry and molecular simulations as practical methods for engineering education and application*

These same issues of chemistry, life sciences, and appropriate tools for modeling them are important at all levels of the profession, from undergraduate curricula to continuing education for practicing engineers. The third approach is taking shape in graduate curricula now, and it will begin to influence undergraduate curricula more as texts begin to appear.

Integrating Molecularly Based Chemistry

The chemistry of chemical engineering is more important than ever, both in established industries and newer industries—from nanostructured materials to biotechnology to process units to atmospheric impact. New physics is also important, certainly for non-Newtonian fluid flows, morphology-property relations, and the solid state. Even there, many of the interesting, relevant issues for chemical engineering physics are molecule-specific and must be dealt with on electronic and molecular scales.

Ironically, chemistry has been dis-integrated from engineering courses. Ten years ago, a University of Massachusetts senior disparaged required chemistry courses as being "scientific liberal arts—something you had to take because it was good for you, not because you ever used it." This was perception rather than reality, but it was perception based on our failure both to show where chemistry was coming into play and to use more of it in chemical engineering courses.

Why is this linkage poor? In contrast to 1898, where "practical" chemistry courses were the primary type offered, modern chemistry courses are more focused on scientific principles, mainly on the molecular scale. Chemical engineering faculties not only have approved of such changes, but we have also moved the ChE curriculum toward fundamentals, mainly of continuum physics. This has put the profession on a solid intellectual footing and advanced the field. In emphasizing scientific fundamentals, however, it has proven harder to spend as much time or to be as experienced in process-scale applications.

We can easily address some improvements. In transport, thermodynamics, and reaction engineering, it is easiest to teach general principles by using chemical species A and B. It is important, however, to move quickly into problems that require real properties of real chemicals, real mixtures, and real reactions. Using real species is the norm in material and energy balances, separations, process design, and the chemical engineering laboratory. In these courses, we must help the students realize they are applying what they have learned in general chemistry classes about nomenclature, balancing reactions, calculating molecular weight, equilibrium constants, and using the ideal gas law.

To really blend chemical science and application, however, we must work to make sure the right chemistry courses are required and that we then use their content. There are several issues to be remembered.

- *We use much of the general chemistry course content*, the main exception being its molecular perspective on bonding and properties.
- *ChE courses often use little from the organic chemistry courses* except for nomenclature of small organic molecules. Memorizing lists of reactions is usually emphasized in the course, and they are treated nonquantitatively. More constructively, the courses include the role of bonding types in determining molecular structure, properties, and the reactivity manifested in these actions. This perspective should be used much more effectively in the chemical engineering curriculum, which tends to imply that properties can be looked up as needed.
- *Biochemistry is rarely required or used*, but it should be.
- *From physical chemistry courses, the ChE curriculum mostly uses thermodynamics, kinetics, and the laboratory experience.* Physical chemistry is usually split into a lab and two or three courses. The first course may contain some kinetics and reaction equilibrium, but it is largely redundant with chemical engineering thermodynamics. This redundancy is normally argued as necessary for students to master this difficult subject. ChE students, however, often gain comfort with thermodynamics through using it, as in equilibrium separations, rather than in restudying the fundamentals.

  Some schools have reasonably made the physical chemistry thermodynamics course optional. Unfortunately, the traditional second physical chemistry course—quantum mechanics, spectroscopy, or possibly some statistical mechanics—is usually perceived to be an easier course to sacrifice. This feeling arises because it is often taught as a narrow and purely intellectual subject, disconnected from relevance to applications. Seeking to adapt present courses in coordination with chemistry colleagues is important, especially in the short-term. Chemical engineers, however, must ultimately take responsibility for integrating physical chemistry and engineering content.

Molecular structure is the basis of many chemical and physical properties which can be estimated, correlated, and sometimes calculated, beginning from simple descriptions of molecular structure. This does not necessarily require computational chemistry, although computer models can help. In ChE courses, molecular structure and properties can be related to common engineering properties such as activation energies, heat of mixing, vapor pressure, thermal conductivity, or free energy of formation. Quantitative estimates of properties are even more convincing. For example, when students know the atom connectivity in a molecule, they can generate quite useful activity coefficients and ideal-gas thermochemistry from UNIFAC and Benson group-additivity methods, respectively.

Reaction engineering provides many good examples of molecular-level processes that have reactor-scale impact. For example, reaction chemistry is inherently molecule-based. Individual molecules react, although collective behaviors like solvation and conduction bands in catalysts influence the reactions. Even so, solvation involves localized shells of solvating molecules and is dominated by solvent-molecule coupling or shielding between solvated molecules. Conduction bands represent the populations of occupied and unoccupied orbitals. This information must be turned into rate expressions and rate constants, or rate constants may be organized on the basis of patterns in the molecular information. Semi-quantitatively, reactions can be classified logically by molecularly general and specific transition states

- *As s,p-orbital reactions*—radical reactions of association/dissociation and abstraction, ionic reactions, and pericyclic reactions
- *As d-orbital reactions*—reactions based on the *d* orbitals of metals, including adsorption and catalysis.

Quantitative Structure-Activity Relations (QSARs) are further examples, where molecular parameters (often using computed values) are used in fitted correlations of rate data.

Chemical engineers excel at combining chemical kinetics with all the other phenomena occurring in chemical processes. Many of these phenomena—such as thermochemistry and chemical equilibrium, phase equilibrium, and most transport processes—have meaning only for domains that are large enough to be statistical continua. The continuum relations, however, are determined by intermolecular interactions, which, in turn, are determined by the shapes and structures of the molecules (the masses and nuclear positions of their atoms and their electronic structure).

Teaching chemical engineers about these relationships and how to exploit their understanding cannot be relegated to science courses. Rather, existing and newly-developed ChE courses and texts must integrate these molecular-scale relations with continuum-scale relations. In this way, real reaction chemistry and property relations can be understood and used effectively. For over twenty years, Preetinder Virk of MIT taught a graduate course in physical organic chemistry titled, "Industrial Chemistry," developed as an updating of the traditional industrial chemistry courses. It has been very successful in convincing students that they could apply chemical principles quantitatively.

Incorporating Life Sciences into ChE

These arguments also apply to understanding and using the chemistry of life sciences. Biology is dramatically increasing in importance. For classically prepared chemical engineers, biotechnology is a logical extension of reaction engineering and separations. This is not the biology of classifying genus and species, however, but of biochemistry, microbiology, and increasingly, molecular biology. Molecular-scale underpinnings of these life sciences are rapidly becoming more understood qualitatively and quantitatively.

Biotechnology has eagerly sought chemical engineers, valuing the profession's classical reaction and separations skills. The ongoing transformation of life sciences toward chemistry and informatics makes them naturals for chemical engineers also. However, few chemical engineering curricula require any microbiology, biochemistry or molecular biology. The life sciences are reasonably accepted as being inside the tent of ChE academic research, but they are mostly omitted from the curriculum and forced to be optional or possibly offered as electives.

The challenge is in the details of implementation. The simplest step is to add a biochemistry course, while courses in microbiology and in cellular and molecular biology are valuable, too. All of these courses are fundamental science courses, so merely requiring students to take such courses does not make the subject matter part of chemical engineering. Chemical engineering courses must incorporate this science, just as they do physics or physical chemistry.

Curricula are crowded, and a reasonable zero-sum approach is to substitute biochemistry for the traditional first physical chemistry course in classical thermodynamics. That choice is controversial, but seems justified. Some schools have already adopted this approach.

Another good choice that some departments have made is to add an elective survey course that groups relevant life-science topics. That approach presently requires a specialist in the field, in part for lack of sufficient experience in the field by the other faculty. Lack of an authoritative but usable text can also prevent the scientific rigor or breadth that is needed, depending on the specific expertise of the instructor. Creating an applied life sciences course is the right direction to go, but the course cannot become part of the standard set of ChE courses so long as only a specialist can teach it. Compare this situation to the status of process design or process control courses. They have been specialized areas, but now can be taught by most faculty with chemical engineering backgrounds. The reason is the existence of good texts such as those by Douglas,[9] Ogunnaike and Ray,[10] and Seborg, Edgar, and Mellichamp.[11]

What is needed more is a required, chemical-engineering-oriented course in applied life sciences—taking advantage of the latest advances in molecular biology. One of the first texts to fit this need has been *Biochemical Engineering Fundamentals* by Bailey and Ollis.[12] However, it has been mostly used for elective courses in the field, and much has been learned about the chemical foundations of the life sciences in recent years.

In addition, life-sciences applications must be woven through the curriculum. This approach is crucial but well advanced. Consider the teaching of Michaelis-Menten enzyme kinetics in texts such as that of Fogler.[13] Like traditional heterogeneous catalysis, it is based on the idea of kinetic binding and reaction on sites that satisfy a population balance. A useful difference is that the site is specific, well defined, and increasingly well described (*e.g.* the binding site of acetylcholinesterase in Sussman, *et al.*[14]). Thus, it is a better model to introduce modeling of elementary catalysis. Other examples are the pharmacokinetics problems in Ogunnaike and Ray.[10]

Elective status cannot continue. The life sciences are less and less an option for the chemical engineer. Instead, more and more they must become essential parts of his or her education.

Beginning to Teach Molecular Modeling and its Engineering Applications

The right intellectual framework for molecular-scale chemistry is the Schrödinger equation and the equations of statistical mechanics. These relations parallel the importance of continuum equations for transport phenomena.

The tools to exploit this framework are computational quantum chemistry and molecular simulations. The first classification includes *ab-initio* wavefunction methods, electronic density functional theory, and semi-empirical molecular orbital theory—all based on zero-kelvin solutions of the electronic Schrödinger equation. The second includes Newtonian molecular dynamics and Monte Carlo simulations based on parameterized force fields to model intra- and intermolecular interactions, interpreted through statistical mechanics. There are useful direct combinations of quantum mechanics and statistical mechanics as well, such as computer programs for variational transition-state theory and Car-Parrinello *ab-initio* molecular dynamics.

Computational tools for chemistry are beginning to be used industrially for practical prediction[15] and in the chemistry classroom for teaching, but they are not yet used much in chemical engineering courses. They have the potential to transform chemical-engineering chemistry intellectually in the same way that genomics is transforming the life sciences (and may also transform chemical-engineering data handling). In the career span of today's students, these tools will be used routinely to predict and extrapolate properties of chemicals and materials.

They already are the tools of choice for obtaining thermochemistry and for developing new homogeneous organometallic catalysts by calculations of reactivity, coupled to experimental synthesis and benchscale measurements. They are beginning to play an important role for electronic materials. As a future example, these are the natural modeling tools for the developing field of nanotechnology, applications occurring at the scale of nanometers. Covalent bond lengths are on the order of 1Å or 0.1 nm, and individual molecules may be nanometer-sized or much larger. Condensed-phase materials may have larger structures, but their behaviors and even mesoscale morphologies have molecular-scale origins.

These methods are in use for a broad range of applications in the chemical process industries, in pharmaceutical companies, and in materials companies.[15] The number of specialists is small at present, one to 30 people per company. Nonspecialist use of the methods and of the results is increasing rapidly. While basic understanding of its principles and execution is necessary, computational quantum chemistry can deliver reliable molecular structures and properties with increasing ease of implementation and interpretation. Computational molecular simulations are used less heavily in the chemical process industries, but they are very important in product development (especially of drugs) and are becoming worthy companions to analytic theories. Many industrial sectors have begun to employ engineering-style QSAR and QSPR (Quantitative Structure-Property Relations) correlations based on molecular structures and parameters.

Chemistry courses are beginning to use molecular visualization and even computational chemistry as lecture aids and in computer laboratory assignments. Similarly, chemical engineering courses can use visualization to reinforce molecular-scale concepts. Molecular simulations available on the Web or on local computers are valuable aids to convey molecular origins of reaction and continuum behaviors, as well as the relations and properties that result. The chemical origins of biological processes and biocatalysis are powerfully communicated when three-dimensional molecular behaviors can be shown and related to their bases in specific bonding relations.

Beyond their helpfulness for teaching, these tools will increasingly need to be taught as ways in which practicing engineers will obtain engineering properties. Again, the science and its practice must be interwoven. Such material might be taught as part of the chemistry courses, but it will more likely be taught within chemical engineering core courses—paralleling the observation that transport phenomena courses are most effectively taught in chemical engineering, not the physics department. Several such courses are being developed, mostly at the elective graduate level. For example

- *Since 1992, the University of Massachusetts has had a graduate chemical engineering course that couples theoretical and computational tools to engineering applications.*
- *A chemist (Michael Hall) and a chemical engineer (David Ford) co-teach "Computational Chemistry and Molecular Modeling for Engineers" at Texas A&M.*
- *Colorado School of Mines requires its seniors to take "Molecular Perspectives in Chemical Engineering." Molecular modeling is applied in other core ChE classes, and the school's faculty co-teach some of the required physical and organic chemistry courses.*
- *Recently, Charles Musgrave of Stanford has taught a graduate course "Quantum Simulations of Molecules and Materials."*
- *At Notre Dame, Ed Maginn teaches "Molecular Modeling and Theory."*

Course materials are also needed. The Molecular Modeling Task Force (http://zeolites.cqe.nwu.edu/Cache/) of the CACHE Corp., the nonprofit educational software organization, has developed a Web-based textbook on molecular simulations (http://w3press.utk.edu/). In another MMTF project, David Kofke of SUNY-Buffalo and colleagues have developed "Etomica" (http://www.ccr.buffalo.edu/etomica/), a Java-based, visual-programming environment for developing molecular simulations and teaching modules

CONCLUSIONS

The chemical engineering profession must join together in a common vision of how its various disciplines fit together, and the center of that vision should be applied chemistry. This is the most crucial issue for the future of chemical engineering as a profession. Seemingly disparate interests, especially in technologies new to the profession, could yet lead to its Balkanization. Alternately, the profession's present mixture of classical chemical engineers, materials-focused chemical engineers, and biotech- and biomedical-focused chemical engineers has the balance and individual strengths to define, propound, and carry out a new vision effectively.

There are three elements in reaching this vision:

- Integrating molecularly-based chemistry into ChE
- Integrating life science into ChE through its chemical principles
- Beginning to teach molecular modeling and its engineering applications

In chemical engineering education, the undergraduate and graduate curricula must be adapted to this chemistry-centered vision. Engineering curricula have always been under pressure to adapt, but they have been adapted only with difficulty because they are so full. Nevertheless, life sciences and molecular-scale chemistry must be integrated into the curriculum and our self-image of what chemical engineering should mean. The new ABET criteria make such changes more feasible for the undergraduate curriculum. Changing the required graduate curriculum requires a similar deep-seated change in convictions of what the core of chemical engineering is.

Specific near-term curriculum changes can be proposed:

- Course syllabi, examples, and problems should be examined to see that chemical principles are brought out effectively, keeping in mind the molecular perspective of modern chemistry
- Physical chemistry requirements should be re-examined, and its classical thermodynamics course should probably be dropped
- A required undergraduate course in biochemistry should be added
- Students should be able to take courses in microbiology and in cellular and molecular biology
- Elective and required chemical engineering courses should be developed in applied physical chemistry (including molecularly based modeling) and applied life sciences at both the undergraduate and graduate levels. The necessary science applications must be interwoven, as in core chemical engineering courses.

Longer-term curriculum changes can be targeted. Chemical engineering courses in applied life sciences and applied physical chemistry must become part of the core curriculum in order to reflect their principles as being part of the profession's core. If they are core principles, they will also be reflected in other courses. It seems reasonable that computer prediction of chemical engineering properties will become a crucial part of all the courses, especially the capstone design course, so it should eventually become part of the standard curriculum.

To depend on service courses from the science departments is to fail our students. The physics department does not teach the transport phenomena courses to chemical engineering students. Transport is essentially applied physics, yet the engineering-science approach blends fundamental phenomena and mathematics with an application- and process-oriented focus. In the same way, telling chemical engineering students to "go take a course in quantum mechanics," or molecular biology, or something similar, is only to address the scientific half of the issue. It is not reasonable to expect science departments to provide the blend that engineers need. It is up to us to create the right blend through course and textbook development.

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