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THE FUTURE OF CHEMICAL ENGINEERING RESEARCH: COMPLEX SYSTEMS

New Tools, New Outlooks, New Opportunities

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I argue that much of the success of chemical engineering during the period 1960–1980 was due to the adoption and mastering of mathematical tools, tools that opened horizons and helped define the profession. I argue that a similar opportunity is faced today, and that several tools from the area of complex systems, which we can readily embrace and develop, should be part of the standard toolkit of chemical engineering. I argue that the field is ready for this expansion, and that these tools will expand the core, crosslink domains, and open up areas where the profession will have much to contribute. © 2005 American Institute of Chemical Engineers *AIChE J,* 51: 1840–1845, 2005

Setting

During the last few years there has been a widespread sense in academic circles in the U.S. that chemical engineering was facing a crisis. This crisis was brought by introspection, questioning of relevance, balance between core and periphery, fragmentation, disagreements about directions, and many other concerns. The driving force for all this introspection was change; the environment around us was quickly changing and ChE was changing as well — too rapidly according to some, too slowly according to others. Change is inevitable and rapid changes lead to crises. However, with every crisis there are opportunities.

It is with this background of introspection and the fact that the *AIChE J* became 50 years old in 2004, that we organized a symposium at the Annual Meeting of the AIChE in Austin with the title "The Future of Chemical Engineering Research." A 50th anniversary is an opportunity to look back and to plan toward the future. The symposium consisted of three sessions entitled *Fundamentals, Biological Engineering*, and *Complex Systems*. My own article was the closing article of the third session, *Complex Systems*. However, to the extent that I prefaced my presentation with a broad view of the evolution of ChE it may be appropriate reverse the order of presentations and open this series with some general remarks. I take the viewpoint of ChE shared by the leading science-based departments from 1960 onward. The perspective is broad, although clearly from the theory side; the brief examples are things I know best, an admittedly idiosyncratic list and other examples can undoubtedly be used. I make no apologies for broadness. I am aware that my observations — if looked through a lens of detail and completeness — may appear too sweeping. I would argue, however, that if we want to sort out large-scale moves one needs a high-altitude view.

Thesis and Evolution of the Discipline

Let me quickly state my thesis. I argue that much of the success of modern chemical engineering over the period 1960–1980 was due to the adoption and mastering of mathematical tools, and that these tools opened horizons and helped define the profession. I argue that a similar opportunity is faced today and that several physical and mathematical tools in the area of complex systems, which we can readily use and develop, should be part of the standard toolkit of chemical engineering. Lastly, I argue that the field is ripe for this broadening of perspective and that several recent works point in this direction.

Let us first look at how we got where we are today. I argue that in the period 1960 – 1975 modeling was "in," new mathematics was embraced, reaction engineering was at the confluence of all the developments and transport phenomena became the ChE paradigm.[1] It quickly become clear what was core ChE and what was not, what was "in" and what was "out". Peripheral areas were trying to become ChE, e.g. materials science, polymers, biochemical engineering. Some areas were fighting for respectability by adopting core tools, for example, mathematical formalisms in the case of fermentation.

ChE was remarkably successful. We operated in a divergent mode, branching out, opening new fronts, and analyzing as many problems as we could. However, every revolution goes too far and we exhausted (figuratively and literally) some of the initially hot areas. Toward the end, we were operating in a convergent mode, unleashing all the machinery to attack ever more complicated problems. In many areas we solved all the interesting problems and what was left was details.

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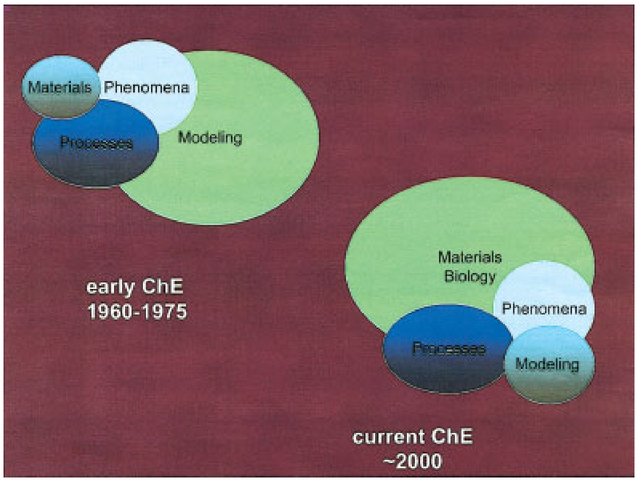

Figure 1. Chemical engineering then and now.

The landscape now is one where biology is central to the picture (Figure 1). We switched from a model where bio and materials were trying to get in to one where chemical engineering departments are struggling to keep all the bio activity under one roof. New all-embracing names were coined: biological, biomolecular, etc. ChE departments gave birth to other departments - biomedical, bioengineering.

How did we get here? In many respects ChE followed the classical mode of growth of organizations, spurts of growth punctuated by crises (Figure 2, adapted from[2]). One cannot talk about the evolution of ChE without connecting it to the birth of the petrochemical industry, and this ties to Schumpeter's waves of innovation and how technologies grow and mature. A long view may be useful. Consider the wave represented by the advent of *water power, textiles, and iron.* This wave lasted approximately 60 years (from 1785–1845), and it was followed by *steam, rail, and steel*, 1845–1900 (55 years), and *electricity, chemicals, and the internal combustion engine*, 1900–1950 (50 years). The birth of modern ChE can be associated with a fourth wave, *petrochemical, electronics, aviation,* 1950–1990 (40 years), and this in turn was followed by the wave of *digital networks, and software,* 1990–2005 (15 years and counting). There is no question that the waves are becoming shorter and shorter. We may now be living in the first half of the bio/nano/info wave, and ChE is trying to ride this wave as well. However, a longer time-horizon is needed. It is clear that tying a discipline to a wave of innovation is not a strategy for long-term vitality. As an example, consider the birth and fate of metallurgical engineering.

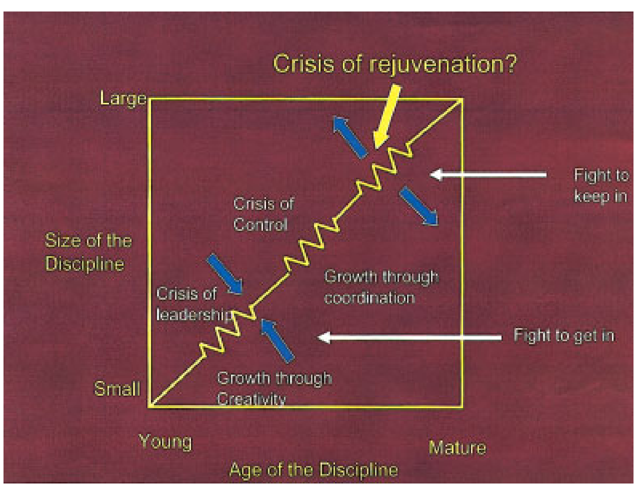

Figure 2. Typical growth of organizations (adapted from reference 2).

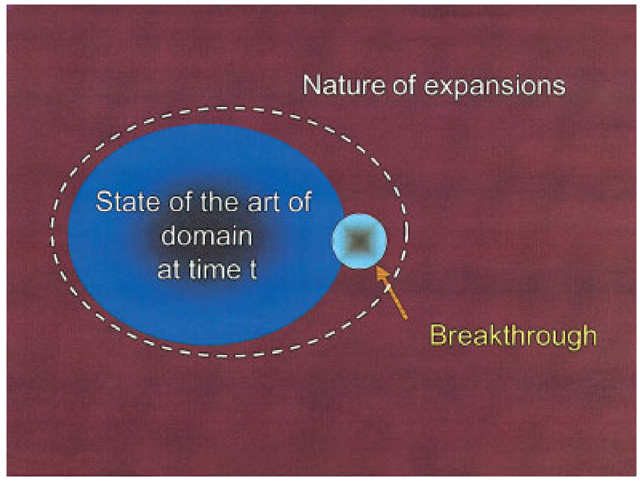

Figure 3. Expansion of disciplines.

A breakthrough results in an augmentation of the state of the art of a domain.

Core-Periphery Interations

Disciplines expand when a peripheral area becomes part of the accepted core of the discipline — think of physics before quantum mechanics, biology before Watson and Crick, electrical engineering before the transistor. Expansion occurs due to *breakthroughs*, addition of knowledge that expands and *breaks through* the boundary of an established domain (Figure 3). They represent also *breakwiths*, since in order to place the new content in the context of the (older) discipline one often has to break with (part of) the accepted dogma of the discipline. However, after integration takes place, the discipline emerges richer and stronger (dashed line in Figure 3). Adding math to ChE in 1960 was such a revolution.

Periphery often remains as periphery; bets do not materialize. Think of synfuels in the late 1970's; in fact, energy is still not a core concept in ChE. Consider other examples; microfluidics represents an augmentation but not a revolution. Environmental issues have stayed at the periphery. Sustainability, still in the periphery, may result in an augmentation of the core. Biology is transforming ChE, but the fundamental integration is still in the works.

In the 1960–1970s ideas flew from the core to periphery. However, since the 1990s the periphery is only loosely connected to the core — a shift from where tools unified the picture to a stage in which the periphery overpowered the core (Figure 4). It may be argued that for many of these peripheral areas the core has become irrelevant. Can the core become relevant again? In order to be so, what should it contain?

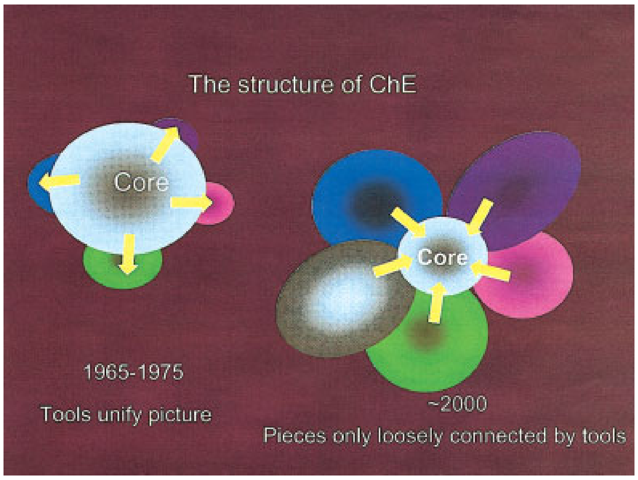

Figure 4. Core-periphery interactions.

In the left figure, the core drives the periphery; in the right figure the periphery dominates.

Hopeful Signs

ChE is highly connected; it has links to chemistry, operations research, many branches of biological sciences and medicine, and all branches of engineering. It may be argued that ChE has the broadest coverage of length scales (see article by Louis Hegedus in this issue[3]). ChE is also intimately associated with a systems viewpoint; and one could in fact argue that the systems viewpoint goes hand in hand with the ability to successfully separate length and time-scales; i.e., break a complicated problem into pieces and then model it by reassembling the whole. Chemical plants can be assembled as a kit, for example. However, there are legitimate ChE problems where decoupling does not work — one can break the problem, but it is hard to put the pieces back and capture the whole. Think for example of all the reactions and transport processes within a cell or a small integrated mini-plant. Many of the recent multiscale and self-assembly problems fall in this class as well.

There is already substantial work in this class of problems and articles in this issue serve as examples. Grossmann's work on enterprise-wide optimization[4] seamlessly merges ChE with operations research; Chris Floudas's article[5] on systems engineering and computational biology places systems engineering as a cornerstone of chemical engineering, with links to computer science, operations research, materials and life sciences. The work by George Stephanopolous and coworkers, a bold augmentation of process systems engineering, represents the launching of the area of nanoscale process systems engineering[6], a manifesto for the design, fabrication and operation of integrated "nanoscale factories" and the integration of units at nanoscales. All this points toward complexity. I believe that these examples represent the tip of the iceberg of what chemical engineering can do.

However, do we have the proper tools in place to give structure to the existing but otherwise dispersed ideas to foster and catalyze further growth? Or to put in the context of core-periphery balance: Should these tools be part of the core of ChE? And if so, what types of "new" problems could become ChE problems?

Complex Systems

What is a complex system? (for reviews see[7,8]). Complex systems can be identified by (1) *What they do* — they display organization without central organizing principle (emergence) — and also by (2) *How they may or may not be analyzed* — decomposing/analyzing subparts does not necessarily give a clue as to the behavior of the whole. Examples of (1) are systems where even if one understood the elementary building blocks, one would not be able to predict the whole, such as neurons and consciousness, or even much simpler problems, such as the emerge of patterns in granular dynamics; examples of (2) are ecological webs.

Complex is different from complicated. The pieces in complicated systems can be well understood in isolation and the whole can be reassembled from its parts. A Boeing 747-400 has, excluding fasteners, 3×10^6 parts. In complicated systems parts work in unison to accomplish a function; pieces are connected to each other according to a blueprint and the blueprint does not change. One key defect (in one of the many critical parts) brings the entire system to a halt. Not so in complex systems; the system may still function if pieces are removed.

Emergence is a central characteristic of complex systems and is intimately related to self-organization and self-assembly and formation of patterns, materials, and so on. In fact, an avenue to the question of "How to make useful patterns or how to make things?" is to rely on self-organization. It is hard to improve on nature in this area. There are however some avenues left, some of them based on traditional tools for chemical engineering and it is appropriate to mention a few. Consider, for example, the micropatterning technique developed by Bartosz Grzybowski and coworkers.[9] This technique is in a sense, equivalent to Guttenberg's printing press — a stamp delivers chemicals ("ink") to a thin film ("article"). The key difference, however, is that here the "ink" does not stay put but migrates according to the system's transport, kinetics and geometry. In one variant of this approach, the thin film is made out of a gel and doped with an inorganic chemical, and a solution of a different chemical(s) is delivered onto its surface from a micropatterned hydrogel stamp. When the chemical from the stamp diffuses into the thin film, it reacts with that contained in the thin film producing a deeply colored precipitate. As the precipitation (color) fronts originating from different features of the stamp approach one another, they exponentially slow down and ultimately leave a sharp clear region between them (see cover photo). Thus, reaction-diffusion evolves a microscopic pattern (tens of microns) into a nanoscopic one (tens of nanometers). The relationship between the shape of the stamp and the resulting nanoscopic image is not trivial — the relationship of one another could be although as akin to a conformal mapping. Variants of the technique can be used to produce simple three-dimensional (3-D) objects[10] and devices.[11]

Another example of self-organization is provided by granular coarsening (see cover photo). Dry and slurry-state granular materials segregate or demix as a result of differences in particle properties, such as density, size, or shape. A particularly interesting case corresponds to long rotating cylinders. In this situation, particles of different sizes quickly segregate into axial bands. Taking a single pixel "slice" parallel to the axis of rotation at the same time over hundreds of rotations allows the creation of space-time representations of the band development. Under some conditions, these bands combine over many revolutions of the tumbler, a process known as coarsening. In other cases traveling waves appear.[12]

Another example, involves small magnetic disks maintained at the interface between a liquid and air or at two close parallel interfaces between air-liquid and liquid-liquid pairs ([13,14]). Disks spin due to the application of a magnetic rotating field. The magnetic field makes the particles move toward each other; however, when the particles get close, hydrodynamics forces become repulsive. This results in a competition between the attractive and repulsive effects, and the particles arrange in lattice-like patterns controlled by an external parameter, the spinning rate of the magnet.

In the coarsening example the pattern can be altered by a forcing parameter, the speed of the cylinder. In the case of the spinning magnetic particles there is one control parameter as well, the speed of the magnet. One can change the strength, but not the qualitative nature of the interactions between the particles. In the stamping example everything happens at once and once the stamp is merged with a given substrate final pattern is unique, although recent work show stamps that can reconfigure themselves depending on the properties of the substrate. Which brings the issue of how to code instructions into the elements of the system and whether or not one can exploit self-organization for practical uses. There are no clear examples of changing the nature of interactions, but these examples undoubtedly will serve as catalysts for much creative thinking. As to practical uses one example where on can see outlines of this mode of thinking in the case of self-assembling mixing[15] and sorting devices.[16] Much of the analysis of these problems can undoubtedly be carried out in terms of existing theoretical tools. However, could we see further by taking a broader view? How can one provide a theoretical foundation to some of these problems? What other problems can one attack?

Toolkit for Complex Systems

The mathematical toolkit of techniques to study complex system studies includes nonlinear dynamics, agent based models, statistical mechanics and network theory. Nonlinear dynamics and chaos in deterministic systems is an integral part of science and engineering; these techniques are common in chemical engineering. Statistical mechanics is also common, although it should be broadened from materials and thermodynamics; recent applications have given rise to new topics, such as econophysics. Agent-based modeling rests on the assumption that some phenomena can and should be modeled directly in terms of computer programs (algorithms) rather than in terms of equations. This type of modeling has started to compete and in many cases replace equation-based approaches in disciplines such as ecology, traffic optimization, supply networks, and behavior-based economics. The inroads in chemical engineering have been minimal. The third element in the toolbox is the newest: network theory. There are reasons to believe that network theory can capture the attention of chemical engineers.[17]

A network is system of nodes with connecting links (Figure 5, based on[18]); once one adopts this viewpoint, networks are everywhere[8,19,20,21]; food webs, a network of species connected by trophic interactions; autonomous nervous systems of complex organisms, a network of neurons connected by synapses; gene regulation networks, a network of genes connected by cross-regulation interactions, protein networks, a network of protein connected by participation in the same protein complexes, metabolic networks, a network of metabolites connected by chemical reactions (see reference[8] for details and full references). Much is known about the architecture of networks and how they form. There are many examples of studies of networks of interest to ChE's, although nearly all studies so far have been published outside chemical engineering. One such example is the topology of web ecosystems, every species in the ecosystem being a node in a network and the existence of a trophic link — i.e., a prey-predator relationship — between two species indicating the existence of a *directed* link between them. Recently, Amaral and coworkers studied the *topology* of food webs from a number of distinct environments — including freshwater habitats, marine-freshwater interfaces, deserts, and tropical islands — and found that this topology may be identical across environments and described by simple analytical expressions.[22,23] In the same spirit, a recent article in *Nature* reports on a study of food webs as transportation networks.[24] The underlying idea is that the directionality of the links (pointing from prey to predator) defines a "flow" of resources — energy, nutrients, prey — between the nodes of the network. Recent results suggest that a *general* treatment of many problems considered in environ-

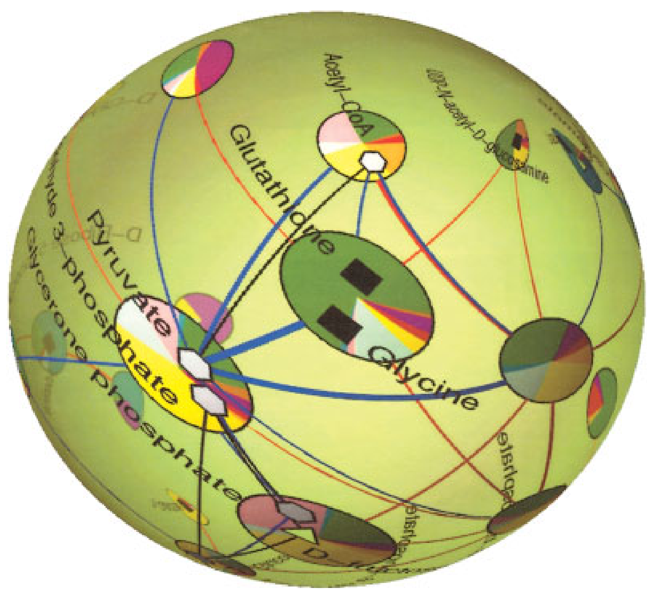

Figure 5. Cartographic representation of the metabolic network of the bacterium E. coli.

The entire network of metabolic reactions in E coli can be grouped into 19 modules, i.e., main pathways. The sixteen most important metabolites, out of the hundreds of metabolites in the network are shown. These most important metabolites are typically conserved across organisms. Figure courtesy of Roger Guimerà and Luis Amaral, based on reference 18.

mental engineering may be within reach. A number of recent studies have started to highlight the existence and complexity of cellular networks. Oltvai, Barabási and coworkers performed a systematic analysis of the metabolic networks of 43 organisms.[25] They found that, despite significant variation in their individual constituents and pathways, these metabolic networks have the same topological scaling properties and show striking similarities to the inherent organization of complex nonbiological systems. Much remains to be understood, but a tentative conclusion is that metabolic organization is not only identical for all living organisms, but also complies with the design principles of robust and error tolerant scale-free networks, and may represent a common blueprint for the large-scale organization of interactions among all cellular constituents. Another important, if formidable problem for chemical engineers, on par with the robustness of the Internet or propagation of epidemics, is the analysis of the petrochemical and chemical supply chain in the U.S.

Conclusions

The long term viability of ChE depends on augmentation of its core, and the opportunity to crosslink existing peripheral domains. A successful rejuvenation of the core will open doors to a new array of problems that would have been unthinkable just a few years ago. The proposal here is augmentation via tools designed to study complex systems such as network theory. Other augmentations are of course possible.

ChE can lead engineering in the complex systems expansion. We are well positioned to venture into ecological problems and systems biology; we are perfectly positioned among engineering disciplines to capture the field of nanoprocess systems engineering; and we must explore the possibility of expanding these ideas to include materials and machine design — situations where self-organization can be part of the design.

The tools proposed here are not and end in themselves. Similar comments could have been made about PDEs, and the math that became adopted by ChE in the 1960s onward[26] the objective was not the math but what one was able do with it.

The expansion of engineering with complex systems tools is far from trivial. Engineering is traditionally about assembling pieces that work in specific ways, optimum design and consistency of operation; the central metaphor is a clock. Complex systems, on the other hand, are about adaptation, self-organization and continuous improvement; the best metaphor may be an ecosystem.[27] For engineering, and in this particular case, ChE, the challenge is the realization that many systems of tremendous national importance—for example, the supply chain of the petrochemical industry — are not the result of a single design but an evolution and merging of designs. In this post 9/11 world, an analysis of the consequences of a catastrophe in a chemical plant and its effects on the entire supply chain need all the tools we can bring to bear.

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