Perspective: AIChE 2010 Institute Lecture

Chemical Engineering in a Complex World: Grand Challenges, Vast Opportunities

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Looking at Ourselves

There is something of a tradition in chemical engineering (ChE) of looking, periodically, at ourselves to assess our past and map out potential future courses.[1,2,3,4] In the current confluence of factors and intertwined grand challenges—energy, global health and quality of life, environment—arising from increased connectedness, speed, and complexity, the evolution of ChE as a discipline remains an active subject of analysis and scholarly discourse. This article takes a long view of chemical engineering—both of where the discipline has been and what opportunities lie ahead, and is based on the author's 2010 Institute lecture. The point of view is academic in character and examines three interrelated issues (a) *how ideas emerge and get accepted*, (b) *how networks of ideas lead to new ideas,* and (c) *how new ideas and tools become integrated within the core of an existing discipline*. I argue that the intersection of ChE with *complex systems thinking,* and *significant, pressing and impactful problems,* is very rich in opportunities and the fertile ground where the future of the discipline will be shaped.

Certain perceptions on the character of ChE, such as the following, are fairly broadly accepted: ChE is compact and coherent, especially when compared with other engineering disciplines; ChE departments are rarely fragmented; and there is a science-based, slow evolving underlying framework that unifies the various components of the discipline and profession. Two aspects of ChE may serve to illustrate the historical coherence of ChE's mainstream: It is almost singular in having three nonspecialized journals (the *AIChE Journal*, *Chemical Engineering Science*, and *Industrial and Engineering Chemistry*); and it is singular as well in that there is still one central meeting servicing all the profession (the AIChE Annual Meeting). On the other hand, one should recognize at the same time that strong centrifugal forces are at play; the bulk of what chemical engineers publish and a large fraction of what they present in conferences—as opposed to what may have happened in, say the 1960s and 1970s—takes place outside of the aforementioned outlets.

Several organized efforts to look at ourselves, benchmark the various components of ChE, and peer into the future, have taken place at various time. Others countries have gone through similar exercises, most notably the UK, on one occasion looking at all branches of engineering.[5] In the USA, restricting the attention to chemical engineering, this effort started in 1987 with the National Research Council (NRC) report, "*Frontiers in Chemical Engineering: Research Needs and Opportunities*," usually referred to as the Amundson report, and more recently in 2007, with the report titled "*Benchmarking the Research Competitiveness of the United States in Chemical Engineering*."[6] This second report, known as the Stephanopoulos report, examines the current status of ChE and how it has evolved in terms of various metrics in a worldwide context, such as publications and impact (full reports available at http://national-academies.org/). The report includes also a survey of perceptions of the US competitive position for various areas within chemical engineering. The picture on the whole is bright, but it was noted that US chemical engineering studies have decidedly moved into the micro, nano, and molecular realms.[7] As a result, macroscopic processes are receiving less attention. This imbalance, the study concluded, could put the US position in certain critical areas at risk. In my view, *systems thinking* is one of them.

In Part 1 of this Perspective, a few terms are first defined and then are used to frame the issues surrounding the evolution of disciplines and analyze the status of ChE today. Part 2—using part of my own work as a point of departure—distills and presents the essential mechanisms of how ideas emerge and gain acceptance in disciplines, and how networks of ideas lead to new ideas, culminating to the

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development of my relationship with complex systems thinking. Finally, in Part 3 an outline of possible opportunities for chemical engineering is given, especially as these are connected with complex systems thinking, tools and methodologies; a natural outgrowth of adopting systems thinking and technologies. Very much like Julio Cortazar's novel, Rayuela,[8] the parts can be read in various sequences. Part 1 can be followed by Part 3, Part 2 can be a standalone, and Part 3, the central message, can be read independently as well.

Ideas are always connected to other ideas and some of the ideas presented in the three parts of this article can be traced back to earlier articles and talks: The first, and earliest, in a Danckwerts Lecture[9] presented in London. Another is a lecture honoring John Bridgwater, presented at Cambridge.[10] Both of those appeared in *Chemical Engineering Science*. Some points appear in a short article organized on occasion of the 75th anniversary of this journal.[11] Lastly, various aspects of the evolution of disciplines are covered at greater length in a long article delivered at the Otto Laporte lecture of the Fluid Dynamics Prize.[12] Several of these articles and related talks can be found at http://mixing.chem-eng.northwestern.edu/and juliomariottino.com. However, what flows well in a presentation full of images many not translate well to a written account. In what follows, I present an abbreviated complementary version of the 2010 Institute lecture at Salt Lake City, including some of the lessons conveyed at the lecture. Inevitably, the months that elapsed between the actual talk and the delivery of this article have added new perspective, and I decided to amplify a few of the original points (the interested reader should view the talk to see how ideas mesh with the larger whole).

Part 1. Defining Terms and Thinking about Disciplines and their Evolution

The past provides a foundation for the future and the current structure of a discipline indicates possible avenues for its future growth and evolution. An analysis of the evolution of disciplines can be framed in terms of several lenses: the sequence of drivers and crises, the types of growth—divergent and convergent, and the balance between emphasis of core components and peripheral and emerging areas.

The Balance between Core Strength and Peripheral Areas. The core is the set of central ideas, the must-have knowledge and set of tools and techniques that define a discipline at a given time. Core is about meeting the needs of the present; periphery is about anticipating the future. Mathematics was in the periphery of ChE in 1950, but was at the core by 1970. Molecular viewpoints were at the periphery in 1960, polymers and materials science were at the periphery in 1970, biochemical engineering in the 1980s, and nano in the 1990s. Now they are all core. What once was periphery may now be core, but not all periphery becomes core.

Convergent and Divergent Growth Modes. The balance and tension between core and periphery is mirrored by another interplay, that between tools and problems: tools and techniques flowing out and opening and capturing new areas on the one hand, and problems flowing in, demanding new tools and new combination of approaches to handle the new problems, on the other. *Transport* migrated into polymer processing and biomedical applications, often expanding into entire new fields and industries, like drug release.[13,14] At the same time making incursions into new areas of biology demanded new tools based on statistical mechanics.[15,16] A related concept about evolution is encapsulated by my own dictum of learning to "*go from simple to complex and from complex to simple*." This applies to people and modes of thinking—it is important to be able to do both well—but applies also to entire disciplines. Going from simple to complex entails starting with a simple picture (which may have taken years to distill to its essence), and studying all consequences until the picture is exhausted. Going from complex to simple is to study phenomena and distill what may have appeared to be dissimilar results into a simple picture or model. The reptation model in polymer physics is a simple picture; its consequences are not. Assembling all the pieces that make up for a model of atmospheric chemistry—knowledge of aerosol chemistry, transport, chemistry, fluid mechanics, etc.—is going from simple pieces into what may be a complex whole.[17] The history of ChE shows that the discipline has been able to do both, although a rough examination may suggest that in the period 1960–1980 ChE exported tools but the core was still a recognizable core; in the period after 1990 ChE migrated outwards. All of this interplay between problems and tools has resulted in ChE covering a broad range of length scales, a true systems perspective (Figure 1). It is probably no exaggeration to claim that, within engineering, ChE is uniquely positioned to understand problems covering a wide spectrum of time and length scales (in a larger setting physics claimed this territory long ago). A critical question that will be addressed later on is the following: Does this approach, putting together wholes by assembling the pieces, succeeds in capturing all important problems relevant to ChE or not?

Growth and Evolution, the Sequences of Drivers and Crises. An-instructive way to follow the evolution of disciplines and, in this case, ChE in particular—is by drawing a parallel with the evolution of organizations, that is, the parallel paths of drivers and distinctive growth stages, with each growth stage followed by a crisis. The drivers of growth are creativity, direction, delegation, coordination, and collaboration; the corresponding crises are crises of leadership, autonomy, control, and red tape. A clear parallel between organizations and disciplines is at the *crises of autonomy* stage—what happens when peripheral ideas are embraced late or acceptance does not occur in a smooth way. Areas fight to get acceptance and to get credibility. However, often this process is slow and may culminate in areas breaking away from the core and forming new disciplines. A case in point is the explosive growth of Biomedical Engineering departments—from about 10 in 1970 to 1980 in 2005—driven in the mid-1990s by the dissolution of the Whitaker foundation, when in a short period of time 30 biomedical engineering programs at various universities in the US were created and a number of capital projects were financed.[18]

Seeing Connectivity and Dynamics in Terms of Networks. Networks capture aspects of the internal structure of disciplines—how disciplines are organized, how different parts are connected to other disciplines, and how they fit in a larger whole (Figures 2, 3, and 4). It is now possible to

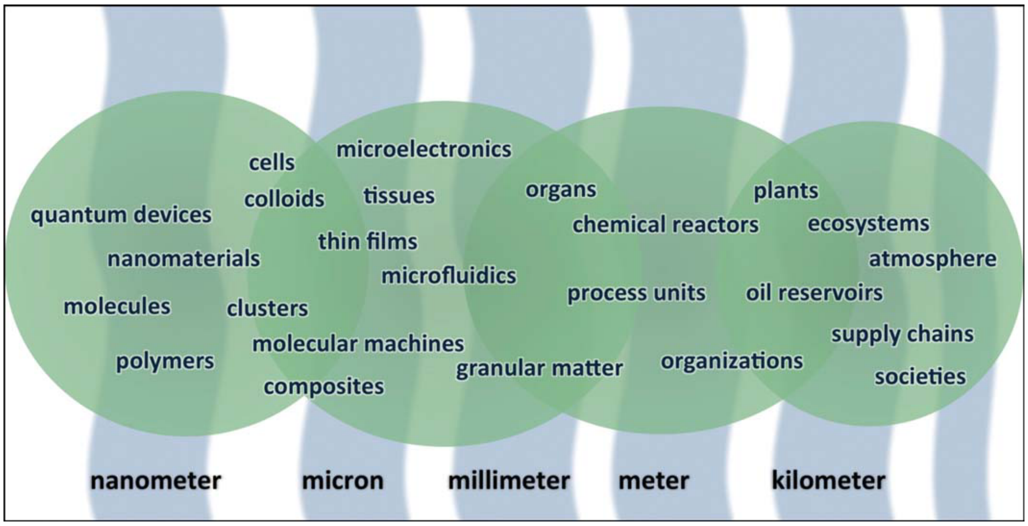

Figure 1. Range of length scales covered by chemical engineering.

investigate how people who publish in specific journals are linked together; how departments within engineering collaborate with each other and with other units within a university. ChE is hardly unique in this respect but the trend is clear: ChE is moving into new areas, connectivity is increasing, and ChE is both exporting ideas and incorporating new ideas from other areas. The examples in Figures 3 and 4 are specific to my own institution, but it is far from atypical and in the case of Northwestern University indicates a temporal strengthening of connections between ChE with chemistry, biology, and medicine, a situation that is anecdotally observed on a national scale. The usual boundaries are becoming insufficient descriptors.

Expansions, Domains, and Fields

Chemical engineering is an example of a *domain*. A domain is the set of all the distilled accumulated knowledge in the form of books, articles, and conference proceedings covering theories, models, experimental evidence, methodologies, schools of thought, etc., in an area of human inquiry. Within a domain there may be subdomains, say fluid mechanics, subdivided into branches such as low Reynolds number flows, turbulence, multiphase flows, and many others; in statistical mechanics, branched into polymer physics, soft matter, etc. In turn, this process can continue where each subdomain may contain sub-subdomains with subdomains, in time, eclipsing the original domains. Domains essentially mirror all the topics covered in major universities.

Domains exist even if people do not. The *field*, on the other hand, is the set of individuals who practice in a given domain. Depending on the domain this may include people in academia and outside academia, in business and government organizations. The expansion of a domain, that is, adding new pieces that become accepted part of the domain, happens at the intersection of the field, the domain itself, and an individual or a set of individuals who act as arbiters or gatekeepers.[19] The field, in a way uniquely self-determined, defines what becomes part of the domain: what goes in and what stays out, what articles get accepted, and what

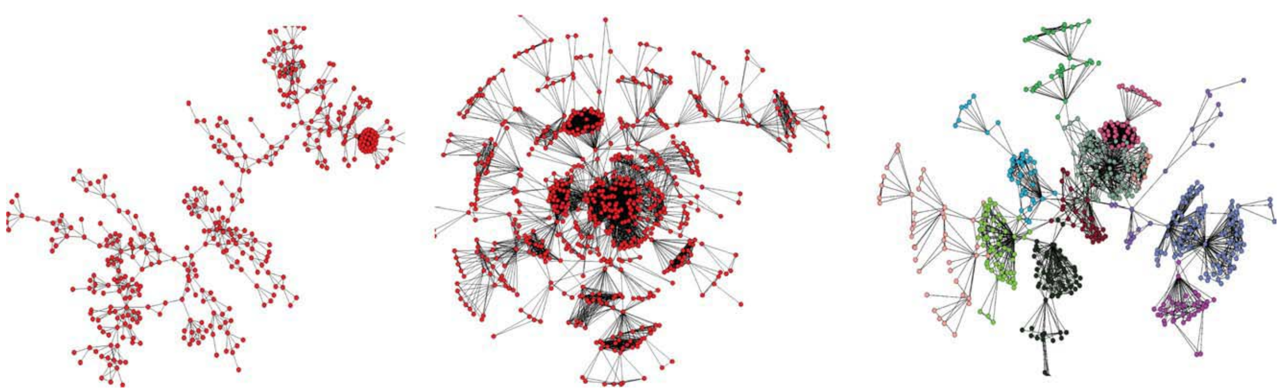

Figure 2. Collaboration in disciplines captured by coauthorship.

Left: Papers published in period 1965–2003 in the Journal of Personality and Social Psychology (9K authors and 8K articles). Center: Collaboration in Astronomy; 11K authors and 13K articles published in the period 1965–2003 published in the Astronomical Journal. Right: Largest connected component of coauthorship within the Dept. of Chemical and Biological Engineering at Northwestern University, showing a network of 600 authors. All figures courtesy of Roger Guimerà.

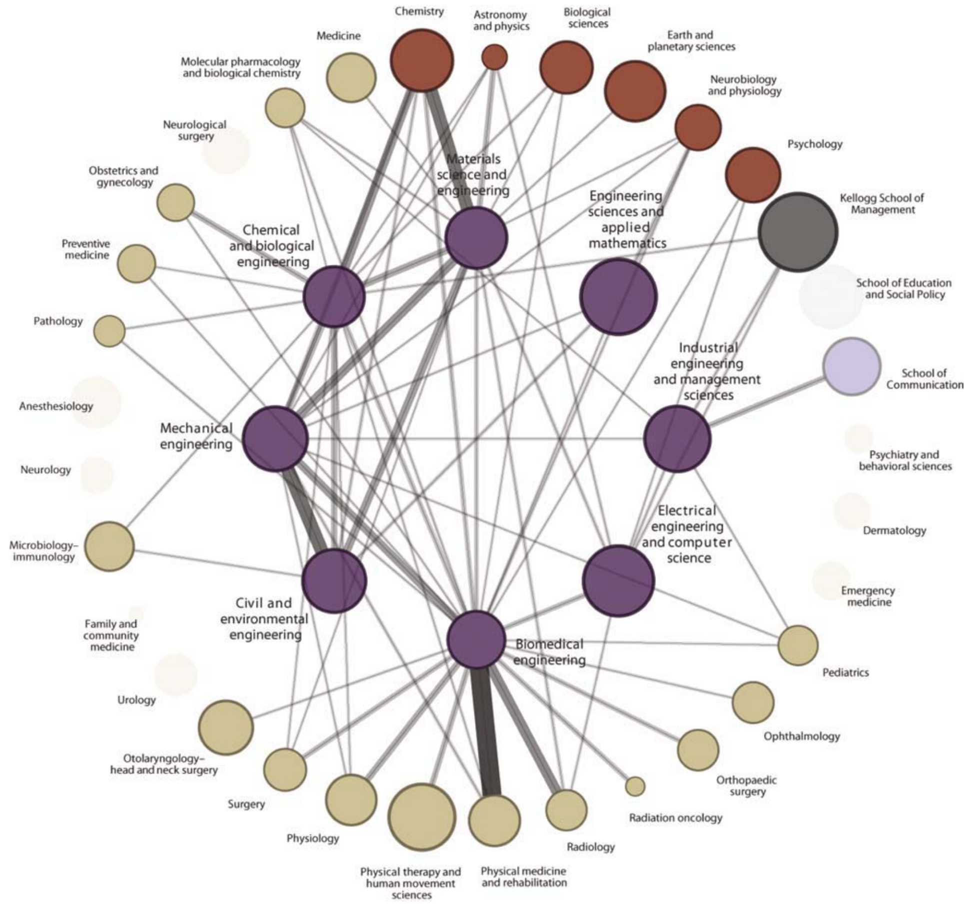

Figure 3. Collaboration within a research university.

The network shows collaboration of various units with the McCormick School of Engineering at Northwestern University in 2010 (inner circle, purple color). Circles represent departments, and the lines connecting two circles indicate that authors from those two departments have collaborated on an article. The size of each circle is proportional to the number of annual publications per coauthor within the department; the thickness of each line is proportional to the number of articles involving authors from both departments. Tan circles represent the Feinberg Medical School; red, departments in Weinberg College of Arts and Sciences; gray, the Kellogg Business School, and light blue, the School of Communication. Faded circles represent departments with no coauthors from McCormick in a given year. For an interactive display of connections, see http://collaboration.mccormick.northwestern.edu/.

ideas may be considered and possibly embraced by the domain. The knowledge-base and structure of a domain itself constrains the kinds of claims and proofs that can be made regarding the acceptance of a new idea. The filter for physics or applied mathematics is different than that for history or economics. All of this happens within a dynamic ecosystem of experimental findings, theories and ideas, with lots of reciprocal relationships; people from discipline A citing works from discipline B and *vice versa* (Figure 5).

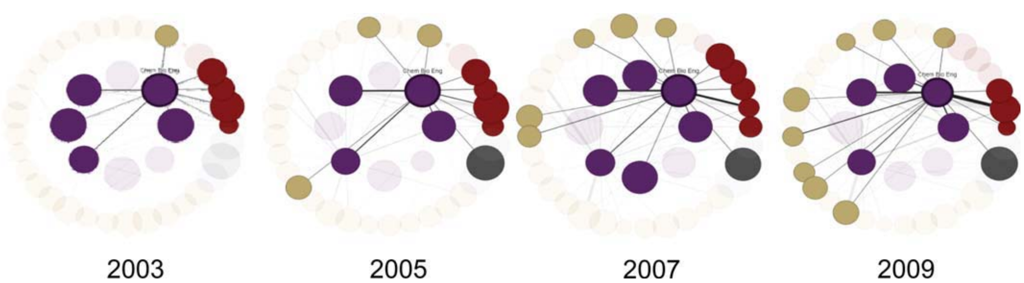

Figure 4. Connections of ChE with engineering departments and other units within a research university.

Circles represent departments, and the lines connecting two circles indicate that authors from those two departments have collaborated on an article at Northwestern University. The size of each circle is proportional to the number of annual publications per coauthor within the department; the thickness of each line is proportional to the number of articles involving authors from both departments. Faded circles represent departments with no coauthors from McCormick in a given year. For an interactive display of connections see http://collaboration.mccormick.northwestern.edu/.

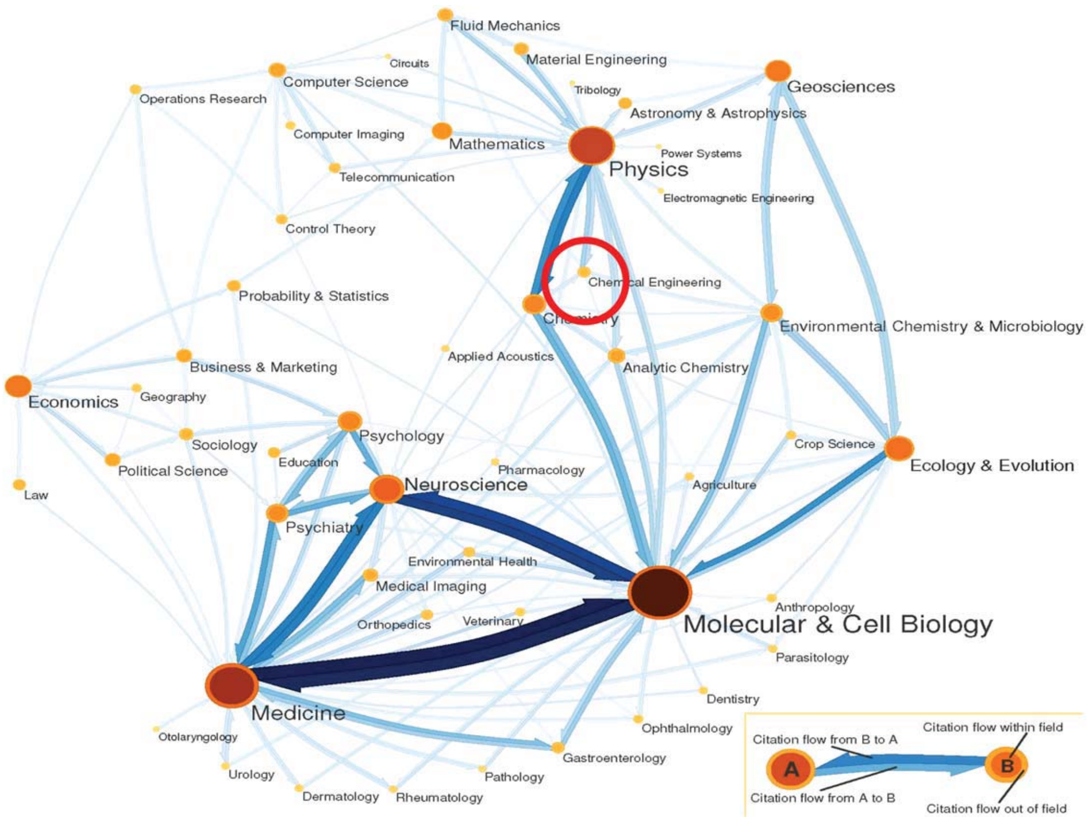

Figure 5. Collaboration across disciplines based on citation flows.

The network covers 6K journals and 6M citations based on 2004 data from ISI. Chemical engineering is denoted by the red circle. Source: Eigenfactor.org.

Domains expand when a peripheral area becomes part of the accepted core of the domain—think of physics before quantum mechanics, biology before Watson and Crick, electrical engineering before the transistor. The addition of significant new knowledge into a domain can sometimes be thought of as a *breakthrough*—an expansion so radical that breaks through the boundary of an established domain. However, some breakthroughs may be better thought of as *break-withs*, since in order to accommodate the new knowledge in the context of (older) knowledge, one often has to break with (part of) the accepted dogma of the discipline. However, after integration takes place, the discipline may emerge richer and stronger. Adding mathematics to ChE in 1960 was such a revolution. It has been said that ''ChE was weighed down with more mathematics that it can actually support.''[20] The comment may be right; revolutions often go too far.

Occasionally a decision by a field can be overturned. This happens rarely in physical and chemical sciences at the level of specific works. It can happen in visual arts—and happens rather frequently—but by definition never happens in pure mathematics. A branch may die due to lack of attention or an emphasis may switch and attention be placed elsewhere. An approach may fall in disfavor, not because the branch is declared wrong, but often because a competing viewpoint gains the upper hand. Even in physical science there may be avenues of pursuit that remain in limbo before the field reaches a collective decision. Water memory, the conjecture that water is capable of retaining a ''memory'' of substances once dissolved in it to arbitrary dilution, Polywater, a hypothetical polymerized form of water, and cold fusion are three examples of areas that failed to become parts of existing domains.

The Picture of ChE

After setting the terms and framework described above, how do we see ChE? By the mid-1970s to 1980s ChE had organized itself around an accepted set of principles, largely science-based, with mathematics and analysis providing the foundation. A core emerged. Clearly this did not happen at the same speed everywhere for all the elements of the core. Starting in the mid-1980s, a number of new areas became gradually fully incorporated within the fabric of ChE, including materials, components of biology and molecular biology, and molecular-based elements. All of these areas had been at the periphery before. Some were early investments, for example, adding courses in biochemical engineering, bacteriology, or statistical mechanics in the 1960s and early 1970s, it took a while before these areas were accepted as a legitimate part of ChE.

ChE was relatively coherent until the mid to late 1980s. The pillars—a list that may include transport phenomena, thermodynamics and statistical mechanics, applied chemistry and catalysis, process engineering, and materials—were well represented in the research programs in a large fraction of

ChE departments (teaching, nearly always, lags behind). The list now includes, on a permanent basis, biological components. However, a second layer of emphasis coexisted and included topics as diverse as electrochemistry and fuel cells, biomaterials, electronic materials and photonics, plasma processing, diagnostics, combustion, oil recovery, colloidal chemistry, membrane science, product design, atmospheric science, and chemistry. This list purposely contains older (e.g., combustion), and newer topics (e.g., biomaterials as in biocompatible materials). The common denominator in the list is that the center of gravity of all these areas resides largely outside ChE. US ChE departments may cover, at most, half of these areas, e.g., air pollution is covered in only a fraction of them. However, in all these cases faculty based within ChE operate at the highest levels of these domains and are often the lead figures on a global scale.

ChE now covers a remarkably wide territory. It is important to note that this broadening occurred even though ChE departments, when compared with other disciplines such as mechanical engineering or electrical engineering, are typically smaller (at least in the US).

However, how robust is ChE now? This question must be addressed in terms of at least two components, ideas and enrollments, but recognizing at the outset that the relationship between the two is far from simple. At time of this publication, undergraduate enrollments in ChE in the US are generally up, but the picture in Europe, with the possible exception of the UK, is far from bullish. The picture in Asia is far from monolithic (Ka Ng, the Hong Kong University of Science and Technology, personal communication). With an expanding economy, countries such as China, India, Malaysia and Indonesia have experienced significant increases in ChE enrollments. Enrollments in developed economies such as Korea, Taiwan, Hong Kong, and Singapore have remained strong, but are relatively steady. The proliferation of new departmental names, such as chemical and biomolecular engineering, chemical and biological engineering, and chemical and environmental engineering, has mirrored that in the US. In this regard, like in many others with potential to affect the world as a whole, China is a significant singularity. The chemical industry in China developed at an amazing speed after 1980 with numbers and challenges that demand worldwide attention. In 2006 coal supplied over 70% of the energy consumed in China; in contrast, the figure for the rest of the world is 20%. The education components are equally eye catching: one-third of all students in China study engineering, the highest number in the world. However, it is also apparent that the economic growth driving enrollment does not necessarily signal added interest in chemical engineering as a profession. There is a significant mismatch between the national importance of the chemical industry and student satisfaction.[21]

It is clear that one cannot talk about the evolution of ChE and its robustness to new ideas without connecting it to surrounding technology. ChE emerged with the birth of the petrochemical industry. It is important to think of this in terms of Schumpeter's waves of innovation and how technologies grow and mature. A long view may be useful. The wave represented by the advent of *water power, textiles, and iron* lasted approximately 60 years (roughly 1775–1845). This 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* (1990–2010, 20 years and counting). There is no question that the waves of innovation are becoming shorter and shorter. We are now living in what may be the middle 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 entirely to a wave of innovation, *and staying with it*, is not a good strategy for long-term viability. As an example consider the birth and fate of metallurgical engineering or what may happen to petroleum engineering.

It is also important to recognize that some ChE bets did not materialize. Periphery often remains as periphery and investments disappear altogether. Think of synfuels in the late 1970s. Microfluidics and microfabrication represented an augmentation but not a revolution. To a large extent, environmental and ecological issues have stayed at the periphery. Energy is emerging, but it is hard to claim strength in energy across the board, especially when compared with other engineering disciplines. Sustainability, still in the periphery, may result in a permanent augmentation. Many of these areas need thought leaders and the establishment of solid intellectual foundations.

In the 1960–1970s ideas flew from the core to the periphery. However, in the 1990s the periphery was only loosely connected to the core–a shift from where tools unified the picture to a stage in which the periphery overpowered the core. ChE, at least in the US, is now emerging from a crisis of rejuvenation.

In many respects a crisis was expected, since it follows the typical growth of organizations.[22] After reaching consolidation there was a widespread sense in the late 1990s in the US that chemical engineering had lost its course and connectivity with its roots. This brought questions of relevance, essentially a discussion about the balance between core and periphery. ChE was changing as well–too rapidly according to some, too slowly according to others. It was argued that for many of these peripheral areas–various forms of bio, nano, etc., were overpowering the core–and that the core had become irrelevant.

The question now is "Can a new core become relevant again?" In order to be so, what should it contain? In three-four decades chemical engineering's reach has expanded from a science-based discipline with a foundation in mathematics and analysis to a broad discipline involving molecular-based elements, materials, biology, and much more. It is my view that ChE can still grow in scope. In fact, there are now tremendous opportunities and a confluence of factors that make ChE more relevant than ever. However, in a curious way this entails going back to our roots and reintegrating and expanding a systems viewpoint.[23] However, before embarking on a discussion of the future opportunities for ChE, let me focus on a few lessons learned about how ideas grow, based on my own experiences in research.

Part 2. Emergence and Acceptance of Ideas: A Window through Specific Examples

Disciplines expand by accepting new ideas, with dynamics dictated by the domain and the field. This is a complex

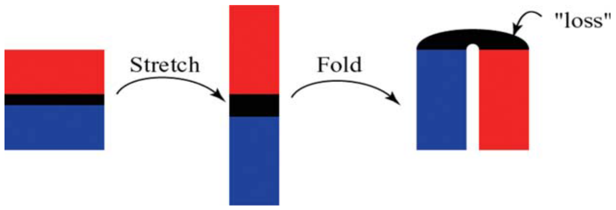

Figure 6. The power of simple pictures—going from simple to complex.

The horseshoe map—stretching and folding captures the essence of mixing and brings with it the mathematical machinery of nonlinear dynamics and chaos.

dynamic process driven by a confluence of factors. The most important learned lessons regarding acceptance and integration are those that have touched us personally. Often through specific examples–our own research, for example–we gain broader vistas and see the broader implications. In this section I try to capture a few of these lessons. A more complete account appears in [9].

Fluid Mixing

The first problem I tackled during my PhD was fluid mixing. In those days it was not a terribly elegant subject, connected mostly with unit operations rather than fundamental fluid dynamics. A point of departure, and one that guided my initial work was the interplay between mixing and chemical reactions.[24] However, in hindsight, I was looking for the essence of the problem, seeing the simplicity within the complexity, the simplest vantage point with maximum implications. The essence, I thought, resided in seeing what happens to an initial condition (IC), a marked piece of fluid, and then looking at a test region and seeing if parts of the IC fall within the test region. Part of the required mathematical machinery was out there—how to quantify deformation and all the machinery coming from continuum mechanics,[25] and maps and iterations of maps, this part coming from pure mathematics—but these two pieces had not been put together. Synthesis of these ideas led to chaotic mixing. A thorny point was to argue that not all problems in fluids should start with the Navier-Stokes equations, and that low Reynolds number flows, long regarded as reversible, could lead to chaos and that the two ideas were in fact compatible. At that point the arguments were kinematical with dynamics emerging much later. However, an even thornier issue was that I was looking at caricatures of problems—seemingly disconnected from actual problems—rather than the real problems faced by industrial applications. The picture of the IC and the test region were connected with deceptively simple looking pictures and a hierarchy of mixing associated with pure mathematics Baker's and horseshoe maps (stretching and folding; an idea that goes back to Osborne Reynolds;[26] see Figure 6).[27] At some point models and experiments entailed identifying regions where a piece of fluid returns to where it started; the starting point was two-dimensional (2-D) time periodic systems, not exactly systems that ever occurred in practice. Furthermore, investigating these systems required sketches; and sketches were not popular either. However, eventually things got to be more and more realistic. Going from the 2-D case to spatially periodic systems helped to make the case for relevance. At some point the right mathematics came along for 3-D cases, along with seeing chaos as a sort of fabric on which processes like breakup, fragmentation, and aggregation could take place.

In retrospect there were two lessons connected to the evolution of these developments that one can distill: (1) Without context it is hard to know where one stands; there was context for what I was doing, but it resided outside ChE. (2) Sometimes the pieces of knowledge do not come ordered in a neatly organized way. For example, it was fairly late when we learned about the Brower fixed point theorem and its guarantee of periodic points when applied to 2-D periodic flows. Sometimes we went backwards; for example, focusing on systems for which one can prove mathematically that they will give rise to the strongest type of mixing over a finite set,[28] or ''discovering'' mathematical tools that were just there, like framing the problem in terms of symmetries.[29] However, in what is a common occurrence, new mathematics leads to new applications.[30]

A Few Broad Lessons

The Adjacent Possible and Multiple Discoveries. It is important to sit at the edge of a domain— the frontier of knowledge—and see what knowledge can be found by peering at the related and unrelated edges of other domains (Figure 7). What new knowledge can be accessed by relatively small steps and extrapolations from existing knowledge? The theoretical biologist Stuart Kauffman has a suggestive name for what one may term first-order combinations reached from the boundary of this edge: ''the adjacent possible''. The adjacent possible can be thought of as a forever-expanding house—opening a door from a room leads to another room, with new doors that may lead to other new rooms. In the case of prebiotic chemistry—Kauffman's motivating point—the adjacent possible defines all those molecular reactions that were directly achievable in the primordial soup. From those chemicals other molecules formed, and from those, others more complex still, unitil hitting something that could self-replicate. Plans, trilobites, sponges, and brains exist outside the circle of possibility of the primordial soup.

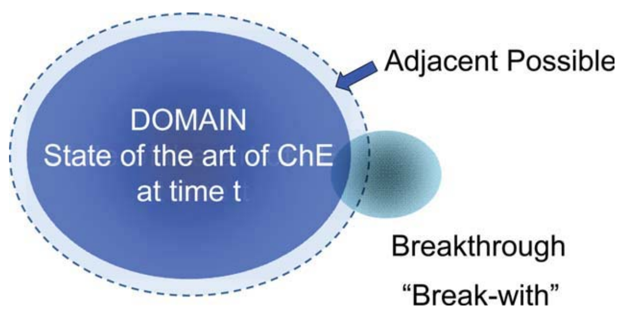

Figure 7. The adjacent possible; ideas reachable from the frontier of knowledge and how expansion of domains happens.

The addition of knowledge is often referred to as breakthroughs; but breakthroughs may often be more properly depicted as a ''break-with'' since the addition of a new idea may require breaking up with previous ideas and beliefs.

The opening of very large number of doors and the visiting many rooms would be needed before reaching a brain.

However, it is important to have a sense of the adjacent possible—to have peripheral vision and to be aware of neighboring, and sometimes distant, disciplines. There is no perfect algorithm for this. In my own case that meant being connected with the latest developments in nonlinear dynamics and the lucky break of connecting with a PhD student pursuing a degree in pure mathematics. The adjacent possible is accessible to the prepared mind and this is at the root of so-called multiple discoveries, people who come up with significant new ideas at virtually the same time. The case of individuals is the clearest. Lord Kelvin is a prime example of this. A Columbia sociologist, Robert K. Merton, and collaborators, examined 400 of Lord Kelvin's 661 scientific communications and addresses and found that at least 32 qualified as multiple discoveries. The co-discoverers were an illustrious set; they included Stokes, Green, Helmholtz, Cavendish, Clausius, Poincaré, Rayleigh, all names associated with significant scientific achievement in their own right. However, the list also included distinguished scientists such as Hankel, Varley, Pfaff, and Lamé, arguably a notch below in the prestige scale. However, this does not diminish Kelvin's greatness. It indicates that it required a considerable number of others top scientists just to duplicate only a subset of the discoveries that Kelvin made. Kelvin was a master in opening doors in the adjacent possible.

However, what applies to individuals applies to disciplines as well. Disciplines develop "cultures", ways of doing things. What at one time may have been revolutionary may lose edge with time. It is easy to evolve into an inward-looking culture. The adjacent possible disappears; and with that the opportunities of gaining new territories.

Pushing Boundaries, Getting Ideas Accepted by a Field. One has to be aware of pushing the envelope too far. There is more needed than just correct logic to get an idea accepted by a domain. For example, to get his ideas about constancy of averages accepted by the physics community, James Clerk Maxwell drew inspiration from Adolphe Quetelet, from what one now would call sociology, who in turn had been trying to describe social interactions with the same level of rigor as Newtonian mechanics. In my own case, the idea of chaos in low Reynolds flows had to fit smoothly with the idea of reversibility in low Reynolds flow. A new idea has to factor in the older prevailing ideas. Some ChE departments bet on bacteriology in the mid 1960s. This was the right bet, but was too early. The obvious fit—or so we thought—was chemical reaction engineering. Acceptance was much smoother once departments became more molecular and molecular biology was seen as a natural extension of an already accepted viewpoint.

Expanding the Adjacent Possible in Chemical Engineering. Technical virtuosity is always an edge, but technical virtuosity has to be accompanied with good taste in selecting problems. I remain convinced that depth accompanied by broadness increases the chances of matching good technique to good problems. Gus Aris of the University of Minnesota was a master in consciously trying to expand the set of the adjacent possible in chemical engineering. I am convinced I was a beneficiary of the culture be created. He instituted a series of broadness seminars, organized around topics like

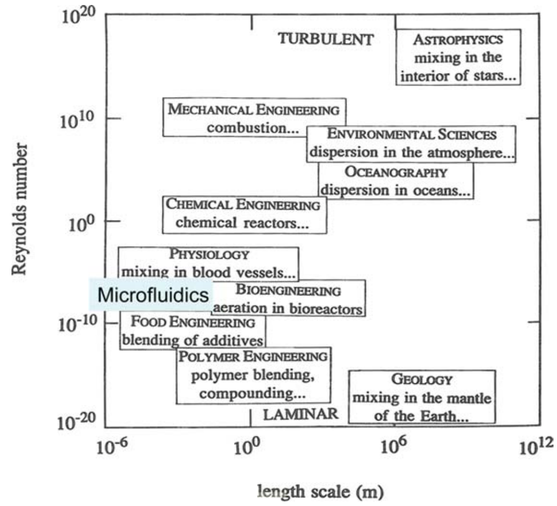

Figure 8. Spectrum of length scales and Reynolds numbers in mixing problems.

Figure adapted from Annual Reviews of Fluid Mechanics.[32]

"elegance". "*That a graduate student should emerge with the title of* '*Doctor of Philosophy*' *without the least contact with modes of thought outside his own field is in the highest degree deplorable…*" Aris said. This ought to be repeated. There are practical consequences of having a wide angle view. For example, I did not know about the t visual and non-visual camps in physical and mathematical sciences, pointed out by Holton, a historian from Harvard.[31] It would have been good or encouraging to know this fact when I was sketching pictures, since the value of sketching pictures was not popular at the time I was sketching mixing trajectories and stretched and folded structures. On the other hand there is something to be said by approaching a problem free of preconceptions and uninfluenced by prior attempts.

At some point ideas become accepted. By 1990 it was easy to predict the expansion of mixing ideas, adding more mathematical sophistication, and seeing how ideas could infiltrate other areas (Figure 8[32]). However, it is nevertheless easy to miss big areas. In 1990 microfluidics was barely part of the adjacent possible. The flip side is that there is such a thing as being too early. The next section touches on this point.

Prematurity and Granular Mixing

Another area of incursion, a natural outgrowth of fluid mixing, was granular mixing. Osborne Reynolds appears here again, his name being associated with unmixing. For this problem, at least initially, a geometric approach worked well[33] with computational approaches coming afterwards.[34] We knew however that we were leaving a lot things out, details at the level of particles themselves, contact forces, for example. All these things came later,[35] including incursions into segregation guided by a kinetic theory viewpoint.[36] Nevertheless the geometric approach proved valuable and allowed us to study the opposite of mixing, unmixing in various kinds of time periodic systems[37]—the unmixing effect or segregation having been something identified by Reynolds more than a century ago.[38] However, as the research program

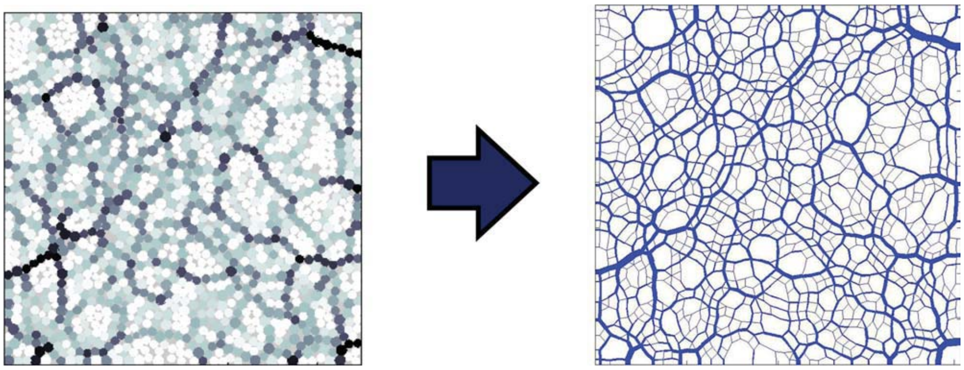

Figure 9. Granular matter as a weighted network.

The left figure represents a 2-D granular system (simulated using soft-particle dynamics). Darker particles experience higher stress. The right figure represents the granular force network, particles correspond to nodes, contacts correspond to edges, and the magnitude of contact force, the edge weight, is represented by the line width.

progressed, the attraction of what we knowingly ignored became our focal point, and we started paying attention to the structure of contact forces—influenced by some beautiful pictures produced by Bob Behringer at Duke University.[39] The emphasis for a short while shifted to problems like distribution of pressure and evolution and disruption of the network of contact forces upon flow (Figure 9).[40,41]

More Broad Lessons

There is Always Something Simpler (and Simple is Good). One has to be prepared for the possibility of surprises coming from disarmingly simple ideas. For me this was the case of piecewise isometries in work in collaboration with Stephen Wiggins from Bristol and Rob Sturman from Leeds in the UK. The modeling of flow of granular materials in 2-D and 3-D tumbled containers consists of modeling a region of thin rapid flow coupled to a region of solid body rotation. An interesting limit is what happens as the thickness of the region of rapid flow becomes thinner and thinner. One could naively expect the problem to be uninteresting since one ends up primarily with solid body rotation. Instead the problem falls in the space of what in mathematics is called piecewise isometries (PWI). PWIs are two and higher dimensional generalizations of interval exchange transformations (IET). An IET is the mathematical equivalent of card shuffling; an interval is subdivided into a number of segments and the transformation acts by permuting the subintervals in a prescribed manner. This leads to *mixing by cutting and shuffling* rather than stretching and folding (Figure 10). However, the problem is also interesting since piecewise isometries lead to "complex dynamics", but with characteristics that do not fit the standard definitions of chaos—for example there is no exponential divergence of initial conditions.[42] The lesson here is in the inherent power of toy examples. Toy examples migrate into books and into teaching—teaching changes perspectives, and changed perspectives bring consequences. Simple examples are especially important to the non-experts who may be teaching a course in areas far removed from their own expertise.

Look for Side Connections. Still there were things for which geometry was not the entry point, and unmixing in long tubes is a prime example. In 1939, a Japanese researcher, Yositisi Oyama, wrote an article that dealt with mixing of two granular materials in a rotating cylinder.[43] The goal of Oyama's work was mixing, but Oyama noted that the materials, when looked from the end of his container, segregated in alternating bands, something that now is referred to as *axial segregation*. This fits the definition of premature— Oyama himself did not regard axial segregation as important or as the beginning of something interesting; now, however, there are hundreds of articles investigating this phenomenon, as it connects with the broad area of pattern formation. However, at the time of Oyama's findings his results could not be connected to any other existing research and the article remained hidden from view. To me, and many others, the segregated patterns had a flavor of cellular automata and this became even more suggestive when long-time experiments revealed coarsening and travelling waves.[44] In turn, the segregation results made me recall what up to then had been a completely unconnected work: Thomas Schelling and his work on segregation in cities,[45] which would result in a book titled "*From Micromotives to Macrobehavior*" (Thomas Schelling won the Nobel Prize in Economics in 2005).

All of the aforementioned tries to exemplify— based on my own limited experience —how ideas emerge, with parts moving in nonsequential fashion, until two or three ideas that had been disconnected appear to be part of a larger whole. The cellular automata viewpoint yielded some results,[46] but the approach did not branch out and reached, at least for us, an end-point. However, more significant was that *three streams of thought that had emerged independently*—the *nonlinear dynamics* connected with mixing, the *networks* encountered in granular matter and the *cellular automata*-like patterns of segregating and coarsening granular matter—were pieces of a broader concept. They were in fact part of something much bigger: the world of complex systems.

Part 3. Complex Systems Thinking

Complex systems thinking should be part of ChE. There are two reasons for this suggestion: First, that complex system thinking is a natural outgrowth in the evolution of the toolkit of ChE. Second, there is confluence of factors and important

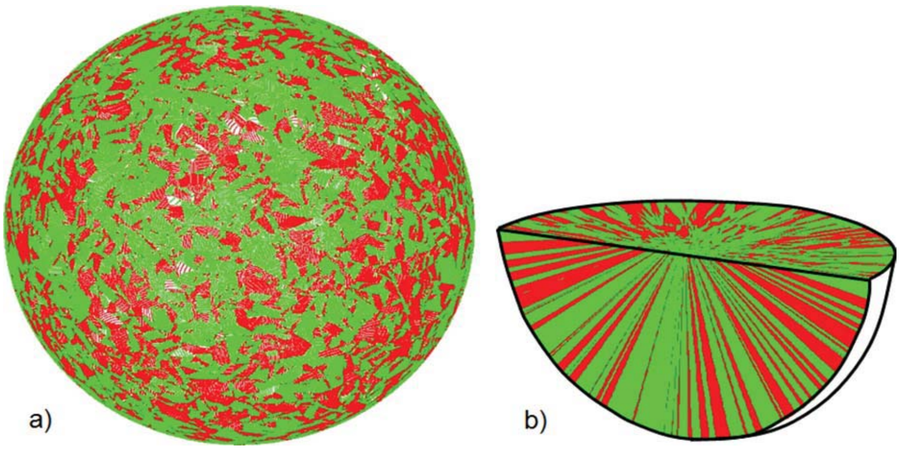

Figure 10. Mixing by cutting and shuffling.

The mathematical framework of piecewise isometries provides an underlying kinematical description of the mixing. (a) bottom view of cut and shuffled structures, and (b) a cut showing the interior.[42]

problems—energy, global health, environment—arising from increased connectedness and complexity. The intersection of problems, complex systems, and chemical engineering is quite extensive in scope and promise. The viewpoint advocated here is to place complex systems tools at the very core of ChE (see [47] for a review of complex systems).

The challenge one faces in the modern world of ChE is successful integration. A point of departure could be process systems engineering (PSE).[48,49]

Systems thinking should be widespread within ChE, but it is not. With few exceptions (Carnegie-Mellon, MIT, Georgia Tech, Princeton, Purdue, Rutgers, and Wisconsin come to mind) ChE is nowadays more connected within campuses with biology, chemistry, and medicine than with industrial engineering, systems engineering, and operations research (OR). It is important to note that OR thinking and complex systems thinking are not a perfect match. PSE is an area with sound mathematical foundations:[50,51,52,53,54] systems dynamics and control, computational optimization network theories, machine learning, artificial intelligence. Complex systems thinking owes more to physics than to mathematical techniques. As a result, while computational optimization thinking can be seen as having penetrated molecular/product design[55,56,57] supply chain/risk management[58,59,60], bio and optimization.[61,62,63,64], it has not penetrated other systems-like areas like ecologies or propagation of epidemics. Areas where the two could meet may include energy/sustainability[65,66] and the transformation of the energy supply chains.[67,68]

One could argue that a systems viewpoint goes hand in hand with the ability to successfully model a system where it is possible to separate length and time scales; i.e., break a complicated problem into pieces and then model it by reassembling the whole. Science rests on the assumption that understanding of building blocks allows the understanding of the entire system. This viewpoint has been remarkably successful and, to some extent, most of the problems covered by PSE fall in this camp. It is becoming increasingly clear, however, that there are limits to this approach. Typical examples of these bounds can be found in many problems of the new fields of interest to chemical engineers, nanotechnology, systems biology, and systems chemistry.

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. It is easy to come up with a long list of deceptively simple systems where the interaction among elementary building blocks does not give a glimpse of the behavior of the system itself, granular matter being one of them. Many multiscale problems fall in the same camp, but multiscale is different from complex; there are complex problems that can hardly be labeled as multiscale. Segregation in cities, as approached by Thomas Shelling, is one example.

Complex systems can be identified by what they do—display organization without a central organizing principle (emergence)—and also by how they may or may not be analyzed—decomposing the system and analyzing subparts does not necessarily give a clue as to the behavior of the whole. Understanding rests on a toolkit that encompasses nonlinear dynamics, statistical mechanics, agent-based models, and network theory.[47]

Complex is also different from complicated (Figure 11). The pieces in complicated systems can be well understood in isolation and the whole can be reassembled from its 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. There are no idle gears in clock, and gears are locked in unchangeable functions. One key defect brings the entire system to a halt. A moon-phase clock, a passenger jet, and nuclear submarine are complicated. So are most chemical plants. There is no adaptation. The way to avert disaster is to back up essential functions, as in a submarine. On the other hand, an ecological system is complex. Within bounds the system adapts; one species may vanish and the system may still be able to function. This indicates that viewing a cell as a sort of chemical plant, rather than as an adaptive system, has limitations as a successful analogy.

Nonlinear dynamics is an integral part of science and engineering and these techniques are common in ChE.

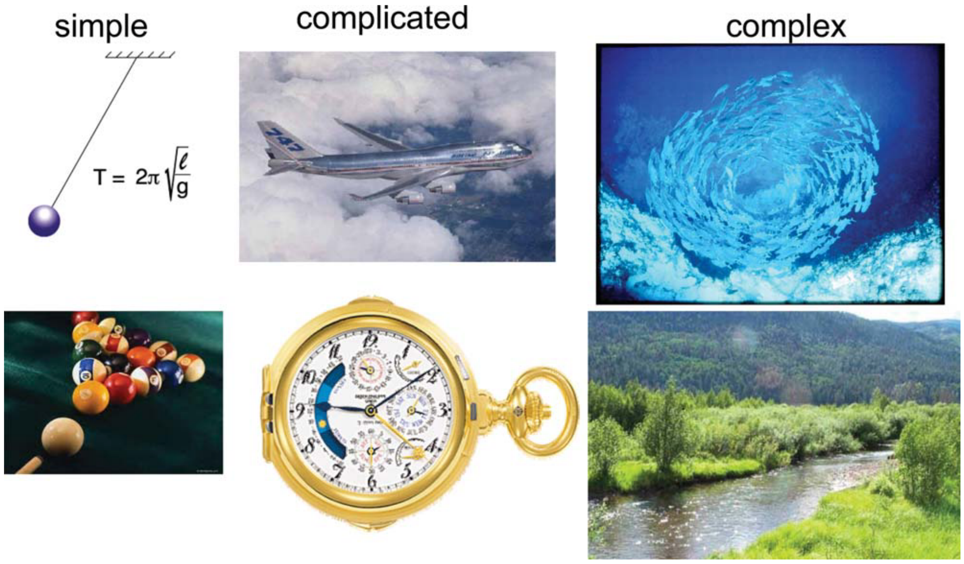

Figure 11. Simple, complicated, and complex.

Simple system are those studied in introductory physics courses; they consist of one or maybe two components, a pendulum or a collision between two balls. Complicated systems involve many parts. In complicated systems parts have to work in unison to accomplish a function. A mechanical watch is complicated. The most "complicated" mechanical watches are called *très compliqué*. They are, as their French name implies, very complicated. A Star Caliber Patek Phillipe has 10^3 pieces. A jetliner is complicated as well. A Boeing 747-400 has, excluding fasteners, 3×10^6 parts. One key defect (in one of the many critical parts) brings the entire system to a halt. This is why redundancy is built into designs of complicated systems when system failure is not an option (e.g., a nuclear submarine). By this definition a chemical plant is also complicated. Ecological systems, the stock market, a termite colony, cities, or the human brain, are complex. The number of parts, e.g., the number of termites in a colony, is not the critical issue. The key characteristic is *adaptability*. The systems respond to external conditions. A food source is obstructed and an ant colony finds a way to go around the object; a few species become extinct and ecosystems manage to adapt. Caution is in order however: The boundary between simple and "complex" is subtle. It takes little for a simple system to become anything but simple. A forced pendulum—with gravity being a periodic function of time—becomes chaotic. A double pendulum—a pendulum hanging from another pendulum—is also chaotic. It does not take much to make billiards within a closed domain become chaotic as well.

Statistical mechanics is also common, although it should be broadened from its roots in materials and thermodynamics; recent applications of statistical mechanics have branched into new subareas like econophysics. The degree of penetration of agent-based modeling (ABM) in engineering has been modest. ABM 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 various aspects of disciplines such as ecology,[69] traffic optimization,[70] supply networks, and behavior-based economics. The third element in the toolbox is the newest: network theory and parts of this has penetrated research in ChE.[71]

Much of the success of modern ChE can be traced to the adoption and mastering of mathematical tools, and that these tools opened horizons and helped define the profession. Some of these tools were connected to systems thinking. However, in the last two decades we drifted away from systems and only about one third of US ChE departments have significant efforts with a clearly identifiable systems component. Bringing systems thinking into the center of the profession can bring significant benefits. However, the viewpoint should be augmented. Systems thinking often means that a whole can be understood by interaction of parts. However, there are many systems where this viewpoint does not work.

Understanding ecological systems should be part of the essential fabric of ChE.[72] However, a food web—a network representation of predator-prey interactions between species in an ecosystem—is one example where decoupling does not work; the problem has to be attacked as a whole (Figure 12). However, "attacked as a whole" does not mean just computing. Ability to compute is not the same as understanding and understanding should be one of the goals.

There are limitations to purely brute force approaches and I encountered several in problems as simple a chaotic mixing.[73,74] A disadvantage to a purely computational attack is that there may be little residual learning—new problem, new attack, and it may be hard to extract conclusions of general value. For example, in the context of a food web, are there aspects that make one food web similar to other food webs? Could some structures of food webs be universal? Some progress has been made on this questions but much more remains to be done.[75] Increasing realism bring formidable problems. So far most of the examples I am familiar with treat ecologies as well-mixed systems. Adding spatial variations may bring issues connected with ABM and even mixing.

Synthetic biology is a new area that brings a formidable set of questions. Synthetic biology[76,77,78] focuses on assembling individual components, engineering organisms unconstrained by biology. However, synthetic biology often leads to unexpected complexity. Biological components (parts), in what may come as no surprise to students of complexity, often behave in a way that depends on the entire system. However, another reason may be the role of fluctuations—components operating at scales and concentrations far below that of Avogadro's number—thus, bringing in the need for stochastic thinking.

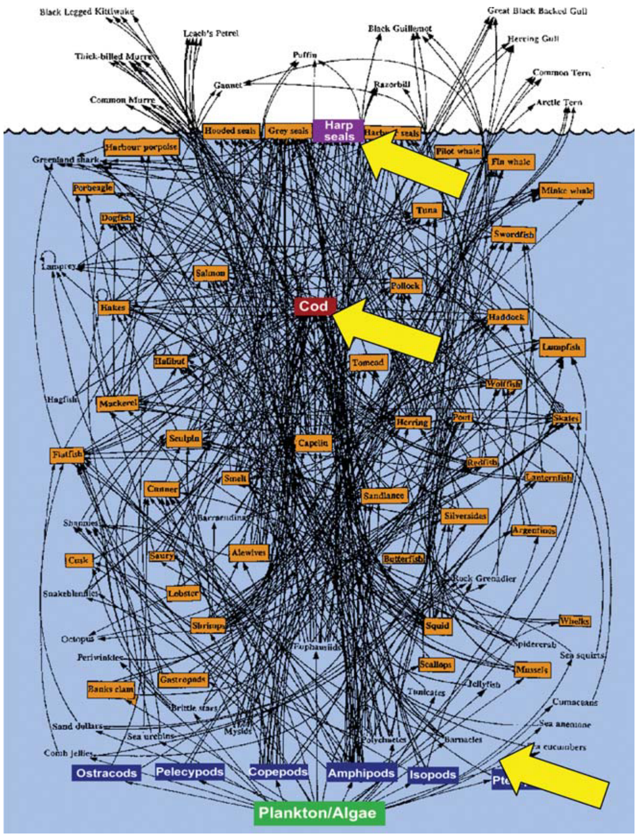

Figure 12. Trophic relationships of species in the North Atlantic.

A naïve predator-prey model would have harp seals eating cod and cod feeding from crustaceans. These three species are indicated by yellow arrows. The entire ecological system is much more complex. Harp seals eat, besides cod, about 150 other species as well. Figure provided by Luis Amaral, Northwestern University.

Similar movement has been recently observed in the newly-defined field of *systems chemistry*.[79] Its range of interests is broad and includes the following: complex molecular networks; catalytic, autocatalytic, self-replicating and self-reproducing systems; dynamic combinatorial chemistry; emergent phenomena in molecular networks; information processing by chemical reactions; bifurcation and chiral symmetry breaking; bottom-up approaches to synthetic biology and chemical evolution; chemical self-organization inspired by the origin and synthesis of life; the conjunction of supramolecular, prebiotic and biomimetic chemistry, theoretical biology, and complex systems physics.

For chemical engineers some of these questions are old and have been tackled by early pioneers of chemical engineering science (e.g., Aris, Danckwerts, Amundson), and those who followed (Ramkrishna, Rudd, Kevrekidis, Klein, Neurock, Feinberg, Hudson, and others). However, most of the aforementioned problems are new and offer a range of vast opportunities for chemical engineers in making long-lasting contributions in unraveling fundamental knowledge on: the creation of self-sustained and self-replicating reaction networks, the foundation of living cells; the principles for engineering nanoscale processes and products; new processes for energy and chemicals production from biomass; and/or novel processes to manufacture a variety of new products.

Networks

A network is a system of nodes with connecting links,[80,81] for example, a food web is species connected by trophic interactions. Once one adopts this viewpoint, networks are everywhere: 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 proteins connected by participation in the same protein complexes; metabolic networks—a network of metabolites connected by chemical reactions. Much has been uncovered in the last decade about the architecture of networks and how they form. There are many examples of studies of networks of interest to ChE's, although it is clear that the bulk of the studies have been published outside of ChE.

Recently, Luis Amaral at Northwestern 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.[82,83] In the same spirit, an article in *Nature* reports on a study of food webs as transportation networks.[84] The underlying idea is that the directionality of the links (pointing from prey to predator) defines a ''flow'' of resources—energy, nutrients, preys—between the nodes of the network. Recent results suggest that a *general* treatment of the problems considered in environmental engineering, with reasonable caveats, may be within reach.

Amaral and coworkers demonstrated that modular networks can be classified into distinct functional classes according to the patterns of role-to-role connections, and that the definition of connection types provides insight into the function and properties of a particular class of networks.[85]

The networks they considered fall into two classes, one comprising metabolic and air transportation networks, and another comprising protein networks and the Internet. The main difference between the two groups is the pattern of connections between nodes in different roles. Specifically, for metabolic and air transportation networks one observes an over-representation (that is, many more than one would expect by chance) of, on the one hand, connections between peripheral nodes and, on the other hand, connections between hubs. In contrast, for protein networks and the Internet one observes an under-representation of those types of connections.

Although it is not possible at present to put forward a theory for the division of the networks into two classes, it may be hypothesized that this could be related to the fact that metabolic and air transportation networks are *transportation* networks, in which strict conservation laws must be fulfilled. Indeed, for transportation systems it has been shown that, under quite general conditions, a hub oligarchy is the most efficient organization.[85] Conversely, both protein networks and the Internet can be seen as information transfer networks, which do not obey classic conservation laws.

Our own incursion in this area focused on cascade failures in metabolic processes within single-celled organisms.[86] Metabolic processes within a cell's interior can be seen as pathways: a series of chemical reactions that transform a starting compound into a final product via a series of small, stepwise chemical changes, with each step in a metabolic route mediated by an enzyme. Our goal was to understand just how robust metabolic pathways are. To gain insight, a comparison was made on how far the errors cascade in pathways found in a variety of single-celled organisms when errors were introduced in randomly generated metabolic pathways. A key finding was that when defects take place in the cell's metabolic pathways, they cascade much shorter distances than when errors occur in random metabolic routes. Metabolic pathways in nature are highly optimized and unusually robust—metabolic networks, far from being haphazardly arranged, are highly organized.

An 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 US. This is topic that has received disproportionally little attention since the pioneering studies of Statdherr and Rudd in the 1970s.[87,88] This is particularly important in light of the evolution of the energy supply in the US.

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 and agent based modeling. The general concept is merging with concepts originating at the very core of chemical engineering and finding support in established figures in the systems area. Stephanopoulos and Reklaitis[24] have observed, ''Through its emphasis on synthetic problems, systems thinking (including complex systems) provides the dialectic complement to the analytical bend of chemical engineering science, thus, establishing the healthy tension between synthesis and analysis; the foundation of any thriving discipline. As a consequence, systems thinking emerges as a foundational underpinning of modern chemical engineering; the one that ensures the discipline's cohesiveness in the years to come''.

The expansion of ChE, and even engineering as whole, with complex systems tools is far from trivial. Some cultural norms are at play. Engineering is traditionally about assembling pieces that work in specific ways and optimizing design and consistency of operation. Complex systems, on the other hand, are about adaptation, self-organization, and continuous improvement.[89]

For engineering, and in this particular case, ChE, the challenge is the realization that many systems of tremendous importance—some, for example, having to do with national security, such as the supply chain of the petrochemical industry—are not the result of a single design but an evolution and merging of designs.

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.

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