Perspective

The Rise and Realization of Molecular Chemical Engineering

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Introduction

Modern chemical engineering involves the integration of physical and chemical phenomena over length scales ranging from the atomic/molecular to the macroscopic. The ability to delve into the molecular world and to learn how to engineer it has opened broad sectors of new technology. How has chemical engineering reached this point? How is chemical engineering taking advantage of this position? How will chemical engineering move forward based on its ability to engineer at the molecular/atomic length scale? In this article, I will provide my biased answers to these questions. Since I will provide my perspective on these issues, I begin by outlining my career in chemical engineering so that my responses can be placed in the context of that portion of chemical engineering history.

I began my undergraduate education in chemical engineering in the early 1970s at the University of Kentucky (UK). At that time, I followed a curriculum that combined the chemical engineering program with a premedical program. The curriculum had very little flexibility because of the large number of required courses. In order to complete this program in four years, I had to overload courses for many semesters and also attend summer school. I did perform an undergraduate research project, and it involved experimental work aimed at understanding a neural network in sea clams under the direction of a professor in biology. After deciding not to attend medical school, I stayed at UK and received both my MS and PhD in chemical engineering. During those years, I concentrated on catalysis and reaction engineering (both experiment and simulation). I began my academic career at Virginia Tech in 1980, and developed an experimental program in the synthesis of highly functional materials. My initial efforts concentrated on synthesizing materials for applications that involved molecular recognition, e.g., catalysis and separations. In 1991, I moved to Caltech where I have continued my efforts in synthesizing highly functional materials, and have expanded the efforts to include materials for medicine. Thus, the window of time through which I have viewed chemical engineering is from the 1970s to the present.

The Rise of Molecular Chemical Engineering

There are at least four key changes that have occurred that have accelerated the rise of chemical engineering at the molecular/atomic level. These key changes are listed in Table 1.

Advances in computers and computation

In the early 1970s, there were still large numbers of people using slide rules for making calculations. However, hand-held calculators were on the rise. Several hand-held calculators with scientific functions were on the market, but their costs were about \$400. (Hand-held calculators with the basic four functions cost much less.) At that time, the scientific calculator costs were significant additions to the tuition cost for in-state students at many public universities, and there were ongoing discussions on banning scientific calculators from tests because they gave unfair advantages to those fortunate enough to have them. When the cost of calculators with scientific functions fell below \$200 these discussions vanished. Personal calculators with scientific functions became commonplace, and homework and exams changed in order to take advantage of this new capability. At that time, computers were large mainframes, and communications with them were via punched cards. All of us who have used punched cards have their own horror stories about using them. I fondly recall having to haul boxes of cards to the computing center and having the entire university computer system (at that time an IBM 370) be dedicated to running my reactor simulations (and, thus, getting very limited time to do so — usually at 2 AM!). Limited numbers of computer terminals with direct access to the mainframe were available, and offered a welcome change to the use of punched cards when one could get access to them.

When I begin my faculty career at Virginia Tech in 1980, I was the first chemical engineering faculty member to have a computer terminal in my office. The terminal had no local

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Table 1. Key Changes that have Accelerated the Rise of Molecular/Atomic Level Chemical Engineering

1.	Advances in computers and computation
2.	Advances in instrumentation to observe molecular/atomic length scales (especially *in situ* methodologies)
3.	Emphasis on bringing synthesis into chemical engineering
4.	A balanced approach to experiment and simulation

computing power and served only to communicate with the campus mainframe (IBM 3032). The ability to do full screen editing seemed like a miracle after using punched cards. At that time, we decided to bring this power to chemical engineering students. Under the guidance of Prof. Peter Rony, we created a computer room for the chemical engineering undergraduate students. Numerous Heathkit computers were purchased and assembled. These computers had a floppy disk drive and 16 K RAM (yes, that is correct — 16 K!). A local computer scientist wrote a screen editing program for us, and Prof. Rony worked with the computing center to network the Heathkit computers so that they could send information to the mainframe and the mainframe could send results back to a printer that we had in the room. I began teaching the students how to use the facility in evening help sessions (they would be able to do screen editing and store their programs on a floppy disk), and we initiated an undergraduate course in numerical analysis. The course notes I developed ultimately became the textbook "Numerical Methods & Modeling for Chemical Engineers."

While this was occurring, the rise of individual computational power was happening. Personal computers such as the Apple II and others were ushering in the initial era of individual computer power. At Virginia Tech, we decided to require all entering engineering students to have personal computers. In 1984, Virginia Tech became the first public institution to implement this requirement. Like with scientific hand-held calculators in the 1970s there was great concern over the additional cost of a $2,000 personal computer to the in-state tuition. The President of Virginia Tech and even the Governor of the state of Virginia stated concern about this. I give a lot of credit to the Dean of the College of Engineering, Paul Torgersen, for believing in the program and implementing it. The personal computer requirement turned out to be a great success, and was embraced by families of the students coming to Virginia Tech. Just like with the implementation of scientific hand-held calculators, the implementation of personal computers allowed significant advances in problems, exams, etc., that could be addressed in the curriculum. Today, all students have laptops and do not even think about the incredible computational power that they now have access to at any time. As I previously mentioned, I used an IBM 370 for reactor simulations in graduate school, and I had to use essentially the complete machine. An IBM 370 had computing speeds of just over 10^6 instructions per second. A modern laptop computer will operate around 10^9 instructions per second, and supercomputers like the IBM Blue Gene operate around 10^{15} instructions per second. This power had a direct influence on the rise and availability of hardware and software for simulating atomic/molecular level phenomena as electrons. Atoms and molecules of sufficient number now can be modeled.

Additionally, in today's world, the amount and speed of access to information is incredible. Because of the advancements in computational power and communications, information and its management tends not to be the bottleneck it was in the past. When I was an undergraduate student, I would have go to the library, search through abstracts and journals to find a scientific article that addressed the question I was seeking to answer. I would then have to write on a sheet of paper results from the paper to take back to the laboratory. Copying machines were just on the verge of becoming readily available for undergraduate student use and that was a large step forward in accumulating scientific information. Today, a student can open his or her laptop, log into the campus library, do an electronic search for scientific information and download a scientific article in a matter of minutes. The amount of information that is available, and the speed at which it can be obtained has changed the way sciences operates. Access to information is no longer rate limiting.

Advances in instrumentation to observe the molecular length scale

Numerous experimental methods and new instrumentation have been developed over the past few decades to observe and manipulate at the molecular length scale. I will provide a few examples. One of the most stunning areas of development was the invention of scanning tunneling microscopy (STM), and atomic force microscopy (AFM). An experiment that caught the attention of not only scientists and engineers but also the public was the spelling of IBM, atom by atom, by D. M. Eigler and E. K. Schweitzer of IBM Almaden in 1989, using an ultra-high-vacuum STM. I have the great pleasure of knowing Don Eigler, and he allowed me to come into his laboratory and move individual atoms shortly after his landmark article was published. This type of work has allowed the manipulation of atoms and molecules and the study of their natural and engineered structures. Insights into local structure and function have been elucidated via these new methods in application areas from electronic materials to catalysts.

High-vacuum surface science matured during this timeframe and has provided useful insights to atomic/molecular structures and their functions. Significant efforts have been made to relate observations made at high vacuum to higher-pressure conditions with some successes. Additionally, methodologies have been and are currently being developed to lessen the requirements for high vacuum so that measurements can be made at conditions closer to real working conditions.

Real advancements have been achieved in the development of instrumentation that can observe the atomic/molecular length scale at *in situ* conditions. Specifically, *in situ* atomic-resolution electron microscopy can now be accomplished. Numerous studies have now appeared using this methodology, and the results are stunning. Additionally, a growing number of facilities that can provide synchrotron radiation are becoming available worldwide. The high energy and monochromatic nature of various focused beams from a synchrotron can be used with techniques such as extended X-ray absorption fine structure (EXAFS), X-ray absorption near edge structure (XANES), X-ray diffraction (XRD), etc., to determine atomic/molecular arrangements, electronics, etc., under working conditions. The ability to probe the atomic/molecular length-scale while the sample is performing its intended functions has occurred only recently, and has provided a whole new understanding of molecular structure and function.

Emphasis on bringing synthesis back into chemical engineering

Chemical engineering drifted away from chemical synthesis as computers became readily available. Molecules became "A" and "B" and the chemical details were often ignored. Advances in computational power and methods provided means for chemical engineering to significantly improve the descriptions of processes and their control. However, in my opinion, the balance between chemical and physical phenomena swung too far away from the chemical side. When I received the Presidential Young Investigator Award from the NSF in 1985, I proposed to use the funds to work on the synthesis of zeolite materials. The project was embraced by industry but a NSF staff member said to me (paraphrased) "Why are you proposing to do synthesis? Chemical engineers do analysis." Additionally, all my efforts to convince the DOE to do catalyst synthesis by design led to one of the DOE staff members saying to me (paraphrased) "Only industrial people do catalyst synthesis, you should be working on the analysis of reaction mechanisms." Fortunately, my research group and a limited number of others in chemical engineering did not listen to these people and helped bring synthesis into mainstream chemical engineering. Today, I do not think that this issue even exists. Thank goodness.

A balanced approach to experiment and simulation

The rapid pace of increasing computational power and methods to exploit that power opened new avenues for theory and simulation. It was very exciting to be in the middle of this rapid advancement and it is easy to see why the field embraced this movement. Simulations were primarily at the continuum level and "A goes to B" — type calculations were common. As mentioned previously, this did lead to difficulties between those working with molecules and those who performed simulations with generic molecules. There was a perceived notion that chemical engineering as a field was experiencing a declining chemical understanding. Often, I would hear this when I would consult with industry, and it was causing separation of those who performed experiments and those who conducted simulations. However, as the ability to simulate at the atomic and molecular level increased, there was a return to chemical understanding as it was necessary for the simulations of this type. In parallel to the movement to atomic and molecular level simulations, there was the ability to observe and manipulate at these length scales (as mentioned previously). The convergence of simulation and experimentation at the atomic and molecular length-scales brought chemical engineering to a much more balanced and appropriate approach to the discipline.

One area where the balanced approach to simulation and experiment at the molecular level has produced a rise in chemical engineering is in bioengineering. I suggest that this is at least the second rise of bioengineering in chemical engineering as in the 1980s there was a similar rise of interest in bioengineering. The difference between the 1980s and now is that the current version of bioengineering is at the atomic/molecular level. That is, it involves molecular level understandings of biological structures and their functions at the level of molecular interactions. The convergence of simulation and experiment at the molecular level is clearly apparent in the current movement of bioengineering.

Molecular Chemical Engineering Has Arrived

Realization of molecular chemical engineering

There is no doubt that chemical engineering at the molecular level is alive and well. Theory and simulations span time scales from femtoseconds to hours, and length scales from the atomic/molecular to the macroscopic (see Figure 1). Experiments and measurements probing the atomic/molecular length scales are becoming more and more routine. Thus, chemical engineering is now molecular chemical engineering. This movement has occurred in more traditional applications like chemical reactors (catalyst active sites to reactor inlet and outlet can be simultaneously approached) and newer applications like using the molecular understanding of how viruses mutate to predict vaccination strategies (work of Prof. M. Deem, Rice University) and engineering targeted nanoparticles (see Figure 2) to deliver small pieces of RNA to tumors in humans as a new approach to treating cancer (my own work).

Formalization of nanotechnology

Nanotechnology came to the forefront in the U.S. around 2001. This is primarily because of the formalization of nanotechnology in the U.S. by the creation of the National Nanotechnology Initiative (NNI). NNI was initiated by the Clinton administration, and President Clinton announced this program in a speech at Caltech on January 21, 2000. He quoted the famous presentation by deceased Caltech physics professor R. Feynman in 1959, "There is plenty of room at the bottom," where Feynman is given credit for being the first person to ask what would happen if we could arrange atoms one by one the way we want them. While I believe that the essence of nanotechnology was already in place, the creation of NNI formalized nanotechnology in the U.S., and it provided a focal point for discussions and funding that did not previously exist. It also raised public awareness of nanotechnology issues (both good and bad). Today, I believe that there is an overemphasis on calling almost everything "nano this and nano that." The overuse of the word nano and some of the associated hyped claims have created a lot of confusion in the eyes of the public. My hope is that this will ultimately decrease and real advancements receive proper acknowledgment. There is no doubt that chemical engineering on the nanoscale is occurring and will lead to new and productive technologies for society. However, it is so overpromised at this point, my hope is that we will not lose public/government interest if true advancements appear moderate in lieu of hyped up anticipated outcomes.

Molecular Chemical Engineering: The Future

Chemical engineering has gone through tremendous diversification over my career. When I entered chemical engineering,

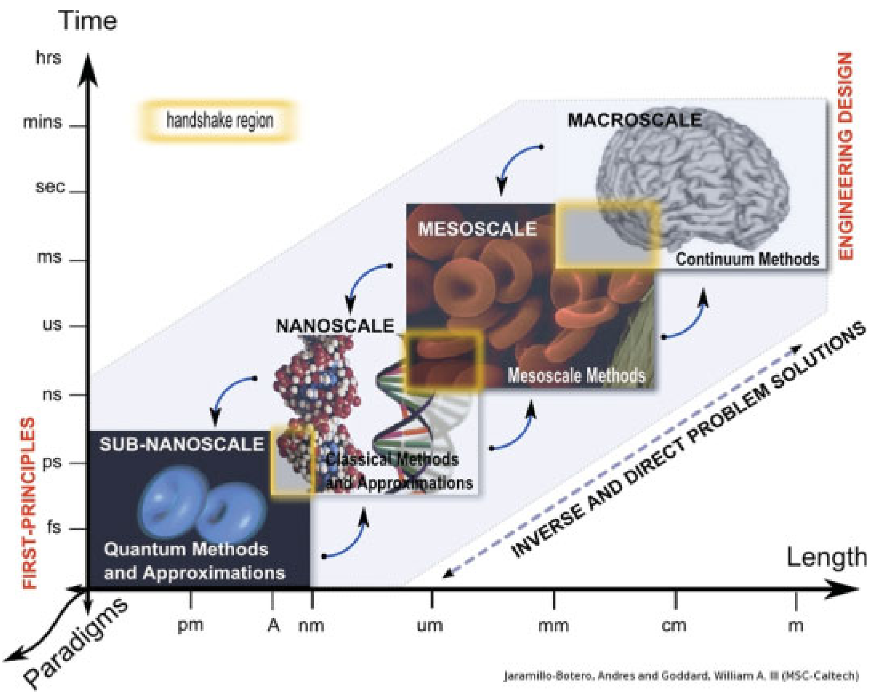

Figure 1. Illustration of the length and time scales now spanned in simulations and experiments.

Figure provided by Andres Jaramillo-Botero and William A. Goddard III, http://www.wag.caltech.edu/multiscale.

it primarily supported the petrochemical industries. Today, graduates populate almost all sectors of commerce. This diversity places demands on chemical engineering education. I list four premises in Table 2 that I believe should be considered. First, the curriculum must be reasonable in terms of requirements and flexibility or it will be difficult to compete for the very best students. The chemical engineering curriculum is typically the most difficult one on campus. While chemical engineering is extremely challenging, it must be convincingly conveyed to students that the payoffs are commensurate with the challenge. Second, emphasis on molecular chemical engineering must be continued and emphasized further as it is the common thread to providing a skill set appropriate for job diversity. Third, modern biology needs to be part of the language of chemical engineering. This education must not be at the expense of chemistry. Since the excitement of modern biology revolves around molecular understandings of biological structure and function, substitution of biology for chemistry is a mistake. Biology should be in addition to the fundamental chemistry as it is the chemistry of biology that is driving modern biology. Also, I strongly believe that it is important to understand that it is the chemical engineering that is brought to biological problems that makes bioengineering have significance. Too much biology at the expense of fundamental chemical engineering is wrong in my opinion. Fourth, professionalism and ethics need to be emphasized to students more now than ever. Engineering has already implemented the teaching of ethics and professionalism to some degree in the curriculum, and I feel that it should be emphasized further. Also, I challenge business schools to do the same. The current economic situation is in large part a consequence of many of the so-called "business leaders" failing to show professionalism. Business schools need to teach the next generation of graduates that a lack of ethical behavior is not acceptable. It is my hope that all educators will join forces to strengthen the concepts of ethical behavior and professional-

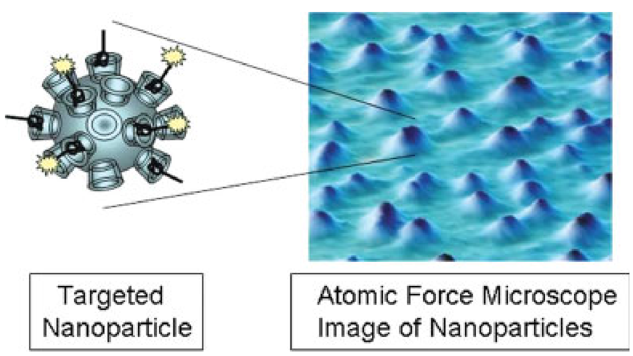

Figure 2. Schematic illustration and atomic force microscope image of targeted nanoparticles carrying small interfering RNAs.

This nanoparticle began use in humans in May 2008 as a treatment for cancer.

Table 2. Key Premises for the Future of Chemical Engineering Education

1. The curriculum must not be overly burdensome in terms of required hours and lack of flexibility
2. The curriculum must provide the essence of chemical engineering and do so with increasing emphasis on molecular level phenomena
3. The curriculum must not ignore biology but also must not replace fundamentals in chemistry and engineering with biology
4. The curriculum must emphasize even further professionalism and ethics

ism in general in the next generation of technical and business leaders.

In order to allow chemical engineering departments to successfully train students for a future career that will have a strong molecular component, I suggested four premises for success that are listed in Table 2. For chemical engineering departments to implement these suggestions and remain accredited, I believe that accrediting requirements and agencies (my own experiences have only been with ABET) need to be overhauled. Current methodologies for accreditation require a significant re-evaluation, as they appear to me to restrict chemical engineering curricula to better serve what chemical engineering was in the past rather than what it needs to be in the future. Modification of the accrediting procedures and requirements cannot be done without the support of the academic and industrial communities. Thus, the chemical engineering community through the AIChE and other avenues needs to actively address and participate in accrediting restructuring so that it can work in concert with chemical engineering departments to meet future goals. To me, a key point that present accrediting procedures do not place sufficient weight on is the fact that chemical engineering is competing for the very best and brightest students, and without them, the discipline will really suffer. We need to provide motivation for the very best young people to join the chemical engineering community by showing them that we are working on the most exciting and important problems for society and by having a curriculum that provides opportunities for them to learn and participate in the most up-to-date, cutting edge science and engineering. These young people demand (as they should) flexibility and freedom to individualize their education. My colleagues and I created a curriculum at Caltech that provides for both a fundamental core of chemical engineering concepts and practices and flexibility. This curriculum is very successful at Caltech.

Modern molecular chemical engineering will need new instructional materials that emphasize atomic/molecular phenomena. The costs of textbooks are rising, while the incentives for faculty members to write good textbooks are declining. Given that authors can now provide electronic files and there is on-demand printing, I do not understand why publishers charge such high prices for textbooks and give such low royalties to authors. (I have written two textbooks in my career, so I have first hand experience with publishers of textbooks.) The situation with the publishers is unlikely to change in the near future, as is the situation with the lack of time for faculty members to write textbooks. Thus, it is unlikely that many new high quality educational materials that emphasize molecular chemical engineering will be available in near future. I offer two suggestions regarding textbooks. First, I would suggest to authors who have textbooks where the copyrights have been returned from the publisher that they provide the texts free of charge on the internet for educational purposes. The Caltech library provides this service, and I have now loaded my two textbooks that are out of print on the Caltech library site for free academic use (M.E. Davis, *Numerical Methods and Modeling for Chemical Engineers* (1984) at http://caltechbook.library.caltech.edu/224/ and M.E. Davis and R.J. Davis, *Fundamentals of Chemical Reaction Engineering* (2003) at http://caltechbook.library.caltech.edu/274/). Other faculty members at Caltech have utilized this service to make their textbooks available also, e.g., R.C. Flagan and J.H. Seinfeld, *Fundamentals of Air Pollution Engineering* (1988) at http://caltechbook.library.caltech.edu/261/. This does not provide a solution to the new textbook issue but does provide a mechanism for lowering the overall textbook cost burden to students. Second, I suggest that the National Science Foundation (NSF) consider creating a funding source for proposals to create educational materials. NSF has increasingly become interested in education and outreach. Thus, the concept of supporting the creation of educational materials is not outside their mission. The idea would be for a group of people to submit a proposal to create an electronic textbook. The main PI would be the editor and numerous investigators could participate in writing chapters. The proposal would provide funds for faculty summer support for writing. The final product would be an electronic textbook free to all for downloading. The electronic textbook could be updated periodically. This idea seeks to address a way to provide support for faculty to create the needed materials and for their dissemination at low (or zero) cost to the students.

Concluding Remarks

I began my career in chemical engineering in 1972 not really knowing what chemical engineering is all about. I am really glad that I made that decision (with the help of Prof. W. Conger in the UK). I have been fortunate to be a part of the rise and realization of molecular chemical engineering. I am excited about the role that molecular chemical engineering can play in attacking the significant societal problems that we currently face. I am proud to be a chemical engineer and I am proud of what chemical engineering has accomplished. I encourage chemical engineers to let the public know what chemical engineering has and will accomplish but do not over-hype. I also strongly defend the fact that the chemical engineering curriculum is the most difficult on campus and that hard work is demanded. However, I also strongly defend the results obtained from this hard work and dedication. Finally, I end with a comment from R. Pausch (the author of The Last Lecture): "If I could only give three words of advice they would be — *tell the truth*. If I got three more words, I'd add *all the time*."