The Evolution of Computing in Chemical Engineering: Perspectives and Future Directions

by

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Introduction

Thank you for that introduction and thanks to the CACHE Trustees for inviting me to speak

It's very gratifying for me to be here 40 years since CACHE was originally founded. Back in 1969 when we had our first meeting at the University of Michigan in Ann Arbor, none of us could have imagined that one day we would be celebrating the 40th anniversary of such a successful organization.

It was good to listen to Warren Seider's presentation recounting the history of CACHE. The transformation that has taken place in chemical engineering computing is pretty amazing as we have gone from: mainframes to the internet, from a printed newsletter to a wiki-enabled website, and from FORTRAN programs to very large sophisticated software packages. In preparation for this trip I also took a good look at the CACHE website. All of the issues of CACHE News were there online starting with Number 1 in 1971 that I prepared. These newsletters chronicle a lot of history.

Before I get started I would like to take this opportunity to thank CACHE for endowing the Chemical Engineering Practice Award of the AIChE and naming it for me. It was very much appreciated and certainly a big surprise. I know the AIChE appreciated the endowment. I especially want to thank Chau-Chyun for leading the effort to raise1 the funds and to the committee who carried it out.

Outline (Slide 2)

This talk is about a look to the future by drawing the experience of the past 40 years. I'm first going to talk about the forces that have driven the evolution of computing in chemical engineering. I will illustrate these forces with a specific case study: the adoption of process simulation and use this as an example to make some general comments about the nature of the value proposition. Finally at the end I'll say a few words about how I see the future of CACHE

The Evolution of Computing in Chemical Engineering (Slide 3)

(Slide 4) Advances in the application of computing have been driven by three primary forces; I’m going to talk about each of them.

The first major driving force is the relentless increase in computing power. The second is our improved ability to model the physical and chemical world. And the third force is the opportunity to bring economic value

(Slide 5) In 1965 Gordon Moore who was co-founder of Intel stated that the number of transistors on an integrated circuit doubles every two years. This has become known as Moore’s law. Another way of saying it is the computing power per unit cost doubles every two years. This relationship has held remarkably well for over four decades and is expected to continue for at least another decade.

(Slide 6) This decrease in the cost of computing power has fueled a remarkable change in the computing environment that many of us here today have experienced personally as we have gone from the mainframe computer to mini computers to PCs and now to the Internet or cloud computing.

The cost of computing was driven so low that a few years ago people began to say that computing was essentially free. Then they began to say that communications cost was so law that bandwidth could be considered free. And, more recently, the cost of large scale storage has dropped so much that in many situations it is no longer a factor

(Slide 7) The second major force driving the application of computing is the improvement in our ability to model the physical and chemical world. The focus on mathematics in chemical engineering over the past few decades has led to better models in fields such as molecular thermodynamics, fluid mechanics and chemical kinetics. Now, these methods are being extended to the biological world. Ultimately we can expect an improved ability to model economic and social systems. All these models represent a combination of first-principles models and statistical models.

(Slide 8) The third major driving force for chemical engineering has been the opportunity to bring economic value to the process industries. The process industries are huge. Their annual revenues exceed $6 trillion. For the most part their products are commodities. They have no control over the cost of their raw materials or the value they can charge for their products – these are set in the open market. The one thing they do have control over is the efficiency with which they convert raw materials to products. And they must continually improve their productivity.

(Slide 9) The process industries take basic raw materials that come from the earth – like gas and oil and coal and process these raw materials through a vast, integrated network of plants to produce products for end users. These products might be fairly simple like gasoline or very complex such as a new drug. But if you can use models to figure out how to make them less expensively or with better properties you can achieve a competitive advantage and increase profits.

(Slide 10) At AspenTech we estimated that in the $6 trillion industry there were $300-500 billion of economic potential in bringing every plant up to the level of the best-in-class and modeling was the key enabling technology to make that happen.

(Slide 11) The increase in computing horsepower came from outside of our industry. The improvements in modeling capability came primarily from academia who developed new models because the problems were intellectually interesting. The drive to create economic value came from within our industry. The first two forces represent a technology push. The third driving force is a market pull.

Crossing the Chasm

(Slide 12) Geoffrey Moore in his book, “Crossing the Chasm, Marketing and Selling High-Tech Products to Mainstream Customers” divided the population of people or companies adopting a new technology into five categories. The Early Adopters are a rare breed of visionaries who have the insight to match an emerging technology to a strategic opportunity … driven by a dream. They are easy to sell to but hard to please. If you succeed with the visionaries you can get a reputation for being a high flyer with a hot product but that is not ultimately where the dollars are.

The Early Majority are pragmatists. They care about the company they are buying from, the quality of the product or service they are getting. Pragmatists won’t buy from you until you are established, yet you can’t get established until they buy from you.

The challenge for most companies and most technologies is to move from the early adopters into the Mainstream which Moore breaks into three segments: The Early Majority, the Late Majority and the Laggards. He refers to this as “Crossing the Chasm.”

(Slide 13) I’m going to give a case study example in a minute to describe the experience that AspenTech and chemical engineering as a profession had in crossing the chasm to the widespread adoption of process simulation.

Case Study: Adoption of Process Simulation

Innovation Phase (1960-1975)

(Slide 14) The early phase of innovation in process simulation took place in the late 1950s and 1960s and was led by innovators in academia such as Paul Shannon then at Purdue and Rudy Motard then at the University of Houston both of whom were founders of CACHE. It also involved innovators in industry like Bob Cavett of Monsanto Dick Hughes originally at Shell and later at the University of Wisconsin. Three of these pioneers, Shannon, Motard, and Hughes were founders of CACHE.

These early innovators were followed by large projects in each major oil and chemical company to develop their own proprietary, in-house process simulator. We had the development of SPECS at Shell, COPE at Exxon, IPES at Union Carbide, FLOWTRAN at Monsanto and at least 15-20 others. One of the most important projects initiated by CACHE in those early days was to make FLOWTRAN available to universities for use in education.

I taught a summer course in MIT from 1969 into the 1980s on modeling, simulation and optimization of chemical processes that was attended by many of the people developing in-house simulation systems. A number of people who were or became CACHE trustees helped me teach the course, including Warren Seider and Bob Seader.

The development of these proprietary in-house systems was a very good example in industry of moving from the innovators to the early adopters. These systems were developed by experts for use by other experts and they ran on a large, central mainframe computer.

Creation of ASPEN (1975-1981)

(Slide 15) In 1973 I saw the opportunity to develop a common, next-generation process simulator at MIT that would be used by the entire industry instead of having individual companies develop their proprietary systems. At that time, MIT was a hotbed of people applying computers to enhance the human ability to solve problems. People were working on computer-aided civil engineering, computer-aided mechanical engineering, and computer-aided electrical engineering. I asked, why not computer-aided chemical engineering?

The timing was right, too. The country was facing the first energy crisis; the MIT Energy Laboratory had been established to enable large interdisciplinary research with collaboration between university and industry. It looked like the country would have to build hundreds of plants to produce “synthetic fuel” from coal to achieve energy independence. So, I got Warren Seider to take a leave from the University of Pennsylvania and spend the 1974-75 academic year at MIT when we wrote the proposal to the Department of Energy to fund the ASPEN Project and the project was funded to begin in 1976.

Our goal was to develop a common simulation system that would be used by many different companies in different locations that could handle solids and would have an integrated cost estimation capability, a very flexible architecture and many other advanced capabilities.

(Slide 16) The Department of Energy funded the project with about $5 million over five years. We recruited key staff members on loan from industry to work on the project. They received their salary from their company and MIT reimbursed their employer. Paul Gallier came from Monsanto as Project Manager; Herb Britt came from Union Carbide and Joe Boston from the University of Toledo as Associate Project Managers. Some of the work was also done at the University of Pennsylvania directed by Warren Seider. Rajeev Gautam (who is now CEO of UOP) did his thesis working for Warren on free energy minimization techniques for solving problems of phase and chemical equilibrium. Chau Chyun Chen (who is presently a CACHE trustee) also did his thesis at MIT on the ASPEN project developing methods for handling the thermodynamics of electrolytes.

We formed an industrial advisory committee with representatives from more than 50 companies.

When the project was finished in 1981 we delivered the ASPEN source code to the Department of Energy and to the companies on the advisory committee each of whom also contributed $30K in financial support. Both of the two commercial software companies, Simulation Sciences and ChemShare participated in the project and received the ASPEN source code. The Department of Energy made a computer tape of the source code available through the Argonne Code Center to anyone who wanted it for a nominal cost. MIT owned the copyright, but DOE had an unlimited license to use it and distribute it to others.

Formation of AspenTech in 1981

(Slide 17) AspenTech was founded as a private company in 1981. I took a leave of absence from MIT to serve as founder and CEO of the company. There were seven other founders all of whom came from the ASPEN Project including Paul Gallier, Herb Britt, Joe Boston and Chau-Chyun Chen who had done his PhD thesis on the project. We got a nonexclusive license from MIT to the ASPEN software with the right to make enhancements and take title to those enhancements.

Our strategy was to offer a commercial version of ASPEN, which we named ASPEN PLUS. Companies could license the software on a “subscription” basis. For $50,000 per year subscribers received support and regular updates to the software. On day one ASPEN PLUS was exactly the same as the public version of ASPEN. We were competing with software that companies could get free from the government. But companies licensed ASPEN PLUS because they knew for a system to be used it needed to be supported and continually updated.

We could not raise venture capital in 1981. The software industry was still in its infancy. Venture capital firms were not impressed with a company whose goal was to sell to the chemical and petroleum industry. They felt these were stodgy, conservative, smokestack industries and besides the founders didn’t have any significant business experience. So we bootstrapped the company with about $1 million from founding employees, private individuals, and a state-financed venture capital group.

Our goal was to develop the ASPEN PLUS software into a commercially viable product and get it adopted by the early adopters. We did this amazingly well. The early adopters were mostly companies, like MW Kellogg and Eastman Kodak who had been active with the ASPEN Project.

But, in 1986 after five years of business and two rounds of seed financing the company was struggling. We hadn't "crossed the chasm" to get the software into widespread use by the mainstream majority. The software was still being used by a relatively small number of experts in each of our customers. These early adopters bought the software because of its technical capabilities.

The company was dangerously short of cash in 1986 when at the last minute we raised $2.9 million in venture capital financing from Advent International.

Crossing the Chasm to Penetrate the Mainstream

(Slide 18) During the period from 1986-1991with adequate financing, the ASPEN software began to penetrate into the mainstream. Early adopters like MW Kellogg, Mitsubishi Chemical and Dow Chemical made a major commitment to use the software broadly in their company. The mainstream adopters bought the software because of its economic value proposition. By crossing the chasm AspenTech overcame a major hurdle.

(Slide 19) AspenTech went on to have a public offering in 1994 and pursued a strategy of going beyond the engineer's desktop into plant operations and supply chain management with integrated solutions that used the same consistent models across the life cycle of a plant. They acquired best-in-class companies and integrated the software. I stepped down as CEO in 2002. AspenTech is still the leading company providing technical software to the chemical and petroleum industry.

(Slide 20) The penetration of process simulation took place over a 50-year period. At the time AspenTech went public in 1994 I estimated that only about 15% of the engineers who could benefit from modeling and simulation were actually doing so.

I presented this case study to illustrate what is required to take a new application of information technology from an idea into a successful product. The critical step is to deliver on a strong economic value proposition. So, now let's talk about what is required to deliver economic value.

(Slide 21) Delivering Value through Application of Information Technology

(Slide 22) Information Technology delivers value primarily by enabling individuals and organizations to make better decisions and implement these decisions consistently through automation. If there are no decisions to be made it is going to be hard to find a way to deliver value. The availability of models and data enable better decisions.

(Slide 23) This diagram shows a typical model. It takes those the decision variables that are free to be selected along with additional data and predicts results. The form of the model may vary from one application to the next.

(Slide 24)

- In Process design, the model is an engineering calculation, the decisions are the equipment sizes and operating conditions and the additional data are updated costs and design constraints
- For production planning, the model is a linear or nonlinear program, the decisions are the amounts of product to produce at each facility and the additional data are the prices and availability of raw materials. The additional data are prices and availability of raw material.
- For advanced process control, the model is an empirical model of the plant obtained from plant tests, the decisions are adjustments in the manipulated variable and the additional data is online measurements from the plant

In the first two examples the decisions are implemented manually – in the last example it is implemented by an automatic control system.

(Slide 25) In 1994, Jim Trainham who was with DuPont at the time said, "If you can't model your process you don't understand it; if you don't understand it you can't improve it; and if you can't improve it you won't e competitive in the 21st century.

Now, I would like to make four observations about using models to deliver value.

(Slide 26) First, consider three technologies at the forefront of adoption today (computational fluid mechanics, molecular modeling, and systems biology). These are three for which CACHE has task forces. I believe they are mostly at the innovation or early adopter stage. To achieve widespread adoption and commercial success they will need to deliver on a strong economic value proposition. The organizations that are commercializing these applications need to articulate how they enable better decisions to be made, what models, data, algorithms and computer coe are needed and how do we get these solutions used. I believe all of these applications are in a technology push mode, driven by an improving ability to model the physical world.

(Slide 27) My second observation relates to future new applications. If I were looking today for a new application of computing that would have a breakthrough impact, I would look for applications responding to a market pull. I would look at some of the big problems of society such as energy, water, food, environment, etc. and ask: "How can information technology enable better decisions and deliver large economic value. Then marshal the models, data, algorithms and computer systems to enable the decisions to be made and implemented.

(Slide 28) The third observation is that there is a big premium on increased modeling accuracy. One of the early success stories around the use of ASPEN PLUS was the example of an engineer who used simulation to devise a separation scheme that eliminated a distillation column from a process design and saved $25 million in capital investment. In order for that engineer to have confidence in his recommendation he had to be convinced he could depend on the results of simulation because a mistake could be career limiting. This put a premium on having accurate models he could depend on.

(Slide 29) There is a shifting paradigm around modeling. The old paradigm was that engineers needed to be able to do quick and dirty calculations preferably on the back of an envelope. The new paradigm is “as accurate as possible.” The old paradigm focused on the value of “know how”. The new paradigm on “know why.” We used to believe in the 80/20 rule that you got 80% of the value from 20% of the work. Now we are looking for six sigma performance.

(Slide 30) My fourth observation relates to the cost of computer software. In the early days companies hesitated to pay annual license fees of $10-20K for software. But, consider the economics: The annual cost of specialized software like a process simulator is typically $10-20K per user. The salary of the professional using it is $100-200K. The value of the right decision made by that professional can be $10-20 million. Therefore there was a strong incentive for companies to provide the most accurate tools available. Instead of asking “How much does the software cost?” companies started asking “How good is it?” and “How can I get more of my engineers using it.

(Slide 31) The Future of CACHE

Now, let me make a few observations about the future of CACHE based on my experience with some very different organizations. I’ll preface these observations with the comment that I am strictly an outsider looking in, I don’t have first-hand experience.

(Slide 32) CACHE has had a Remarkable History. Just to stay in existence as a financially solvent organization, engaging some of the best people in the profession, doing important work is a major challenge itself.

The core mission, “to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession” has remained unchanged for almost 40 years.

But, the activities have changed dramatically from publishing FORTRAN programs to hosting leading conferences and pioneering new applications of modeling. It has task forces addressing new applications such as computational fluid dynamics, molecular modeling and systems biology.

CACHE has found ways to solve some key organizational problems. The addition of industrial trustees, which occurred very early in the history of CACHE was instrumental in achieving the goal of cooperation among universities and industry.

CACHE has found a way of adding new trustees while still retaining a core of long-term trustees.

(Slide 33) CACHE has been entrepreneurial in adding new funding sources: government funding, supporting departments, industrial affiliates,

CACHE has been at the forefront in many areas. The trustees have been thought leaders in the use of computers at the forefront of chemical engineers. Its products are well accepted, the people associated with CACHE are the leaders of the profession, its conferences and programs are prestigious.

The structure as an independent, not-for-profit corporation has served CACHE well.

A very important key to success has been the role of the University of Texas in hosting the executive office of CACHE and the dedication of people like Dave Himmelblau and Tom Edgar.

(Slide 34) CACHE Opportunities for the Future

I think there will be a continuing need to promote cooperation among universities, industry and government in the use of computing in education. Computing and communications technology continue to change.

New technologies have the potential to make big changes in the way education is delivered, research is published, books are written and technical and professional meetings are held.

There will also be a need for next-generation computing tools to address the big problems of tomorrow. The innovation needs to come from academia.

All of these are areas where CACHE can play a big role

(Slide 34) Thank you.