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"Process Engineering in the 21st Century: The Impact of Information Technology"

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Abstract

Much of the progress of process engineering over the past 20 years can be attributed to the continuing advances in digital computing and, more generally, information technology. The reduction in hardware cost and emergence of standard software packages and architectures have greatly increased the productivity of the process engineer. Fundamental mathematical models are becoming available due to an improved understanding of microscopic and molecular behavior, which could ultimately lead to ab initio process design. This will enable design of a process to yield a product with a given set of target properties, predictable environmental impact, and minimum costs. Information technology will also change the way plants are operated in the future. The merging of detailed models for design, operations, and control will ultimately provide a unified view of process engineering. This new process engineering paradigm has implications for chemical engineering education as well.

Introduction

Digital computers have a major influence on our lives and the development of computers is the most important technological advance over the past 40 years. In 1982 John Naisbitt wrote the book Megatrends [1], which predicted that the United States would be transformed from an industrial society to an information society, which in fact has happened. The costs and capabilities of computers in 1968 (see

Table 1) provide an interesting reference point for the significant changes in digital technology. Consider the IBM 7090 as an example of how computers have become affordable: $55,000/month in 1960 to lease it, not own it. This computer is less powerful than the microprocessor in today's video camera.

	Average Monthly Rental (1960 $)	Maximum Core Storage Capacity (in 1000 bits)	Add Time (Micro-sec)	Cards Read Per Min
IBM – 7090	55,000	160	0.004	250
CDC-1604	34,000	32	0.005	1300
DEC-PDP1	2,200	4	0.010	(Tape Input)

Table 1. Computer Performance Indicators (1960)

In the field of computing, Moore's Law has become a frequently quoted benchmark. Moore’s Law states that the speed of computers will double every 18 months; in other words every ten years the speed of computing will essentially increase by about a factor of 100. Moore’s law is driven by the growing number of transistors per chip, which is a measure of the chip’s computing power. That trend has persisted since the 1960s, and technology leaders predict that Moore's Law will hold for at least another ten to twenty years.

Despite the remarkable advances achieved by computers, we also know that computers sometimes can behave strangely or pathologically. I heard a story about four passengers who were riding in an automobile and all of a sudden their car just stopped running. The passengers were a chemical engineer, an electrical engineer, a mechanical engineer and a computer scientist. They began theorizing about the problem with the car. The chemical engineer said, "it must be the combustion system, possibly the air-fuel system, that's why it won’t run. Then the mechanical engineer said, "the drive train is the problem with this car; that's why it's not going anywhere." The electrical engineer said, "No, no, you're wrong, the electrical system has failed, that's why this car isn't running." So the computer scientist considered these remarks and says, "Let's all get out of the car. Then we'll close all the windows and slam the doors, and then open them again. Then we can get in and the car will run just fine.” This story illustrates that computers can exhibit unpredictable behaviors, but sometimes simply restarting them can solve the problem. Even so, the reliability of computers has gone up by at least an order of magnitude during the past decade, and computers are now widely used in mission-critical activities like computer control, automation, and manufacturing.

Mathematical modeling and simulation are important and useful areas of computer application. In the mid 1970s engineers in industry were skeptical of simulation as a valid way to solve manufacturing problems; few people then believed accurate predictions could be obtained from mathematical models. However, today the prevailing view in industry is that it is much less expensive and more reproducible to run simulation experiments than it is to perform repeated experiments involving actual equipment. The confidence level in what can be done with simulation has risen considerably, and this is having a profound influence on the practice of process engineering.

Paradigms for Process Engineering

The traditional paradigm for process engineering as practiced over the last 50 years by chemical engineers is shown in Table 2. There are several stages involved with developing and commercializing a process. The R&D stage involves discovery, usually by chemists, followed by the pilot plant stage. Here chemical engineers scale-up the process to higher production levels. Scale-up can be performed repetitively, moving to higher production levels until eventually there is enough confidence to design the commercial facility. After the commercial facility is designed and constructed, it is possible to carry out process optimization. In the traditional paradigm, the engineer usually waits until the scale-up process is completed and then a process engineering analysis is carried out via detailed simulation. However, a new paradigm is emerging where simulation is performed even at the discovery phase [2].

Here one can use a flowsheeting package, using approximate equipment sizes, and build a model of the process and its economics.

(1) research and development
(2) scale-up, scale-up,…
(3) design of commercial facility
(4) optimization

Table 2. Traditional Paradigm of Process Engineering (1960 - 2000)

This allows the engineer to decide whether further scale-up is warranted. A few companies are using this procedure now. As you progress through the stages of scale-up, the process model is updated, based on the data acquired. This approach may yield a considerable savings both in time to commercialization and in total costs.

Figure 1 illustrates the relationships between these various steps.

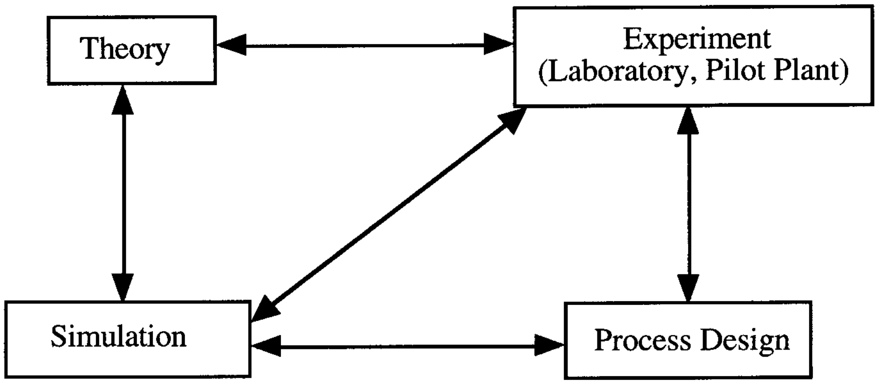

Figure 1. 21st Century Process Engineering Paradigm

The addition of the simulation block in the research, development and commercialization progression demonstrates its importance. The advent of faster computers will enable more detailed modeling that can be performed interactively using advanced analysis and visualization tools. As shown in Figure 1, simulation is not only embedded in the experimental phase but also it is an integral part of theories that rely on intensive computations. In many future engineering calculations (e.g., separation or reaction), structure-property relationships will be derived from first principles that use computer simulation.

Commercial computational fluid dynamics (CFD) packages, such as FLUENT, FIDAP, and NEKTON, can perform a rigorous simulation of flow patterns in a process unit (such as a reactor or exchanger) by solving time-dependent, three dimensional equations of change, in order to analyze and understand the system behavior at a microscopic level. Coupled heat and mass transfer problems can also be solved with CFD codes. Dupont recently reported an application of CFD in a piece of equipment operating in a highly erosive environment that consumed large amounts of steam [3]. CFD modeling showed how the equipment failed on occasion; redesign of the internal components extended the useful life and greatly reduced energy consumption. Tools such as CFD and molecular modeling will someday realize the holy grail called ab initio process design, which means design of an entire chemical plant from first principles. It is a fairly radical notion but one which might actually come to pass in 10 or 15 years. While it is easy to be skeptical about such predictions, I should remind you that no one in the computer business three years ago predicted the stunning impact of the World Wide Web.

In ab initio process design, you stipulate a product with certain target properties. Various flowsheets can be synthesized to find a scheme with predictable environmental impact and minimal cost. In other words, you begin with a set of desired properties and then reverse-engineer the process chemistry and the process design that gives those desired properties. Many biotechnology companies now use molecular modeling tools in drug design to answer questions about electronic structures, chemical properties of candidate molecules, locations of the active sites, and how certain drugs will operate. While I am not suggesting experiments can be eliminated altogether, replacing repetitive experiments with simulation will drive the cost of process development down.

Examples of molecular modeling utility include the prediction of thermochemistry to determine feasible reaction pathways, prediction of spectroscopic properties to enable identification of chemical species that might be involved in determining environmental impact, and electronic structure calculations to provide insights on bonding energies. Professor Gasem at Oklahoma State is now using molecular simulation to predict some VLE (vapor-liquid equilibrium) properties from first principles; VLE properties normally require experimental data and are based on empirical correlations. A current limitation of molecular modeling approaches is the availability of fast computers (in some cases supercomputers) to carry out rigorous computations. To fully develop the potential of molecular modeling, a petaflop (10^{15} flops or floating point operations per second) machine may be needed ultimately. The fastest machine available in the year 2000 at the San Diego Supercomputer Center, one of two leading academic facilities for computing, will be around one teraflop (10^{12} flops). Assuming that Moore's Law will continue to be valid, supercomputers are expected to exceed the petaflop benchmark by 2020. A 233 mhz Pentium PC available today has a rating of about 50 megaflops, or 0.05 gigaflop (5×10^{-5} teraflop or 5×10^{-9} petaflop), so a cluster of one thousand PC's run in a parallel computing mode could approach the computing power of what are called supercomputers today, and provide the computational horsepower needed to solve such modeling problems. Using the same scaling argument, the engineering workstation in 2020 may approach one teraflop in speed.

Dr. George Keller, who recently retired from Union Carbide, has recently co-authored a paper on the future challenges of process engineering [2]. In order for the chemical industry to be globally competitive in the 21st century, process engineers must reduce raw material costs, capital investment, plant energy consumption, inventory in the plant, and the amount of pollutants generated. Keller and Bryan [2] also indicate that the process industries in the future will need improved process flexibility, safety, and control technology.

	% Sales Price	
Item	$<10^7$ lb/yr	$>10^8$ lb/yr
Raw Materials	5-20	40-70
Capital Cost, Including ROI and Depreciation	5-30	25-50
Labor + Fixed Costs	10-50	<10
Energy	5-30	<10
Maintenance, etc.	10-30	<10

Source: Keller and Bryan (1999).

Table 3. Cost Breakdown for Chemical Production

Table 3 [2] indicates for different sized plants the relative importance of various cost categories calculated as a percentage of sales price. For smaller sized plants (typically batch processes), 5 to 20 percent of the selling price is due to raw materials and 5 to 30 percent is capital cost. In larger plants, which generally are continuous plants, the percentages change quite significantly. For these plants raw materials cost and capital cost dominate the sales price. In batch plants, labor and inventory storage costs are responsible for a much larger portion of the selling price. For large, continuous plants, clearly engineers should focus on the raw material costs and the capital costs. What can be done with new technology to reduce raw material costs? Keller and Bryan suggest options such as new reaction pathways, using catalysts to obtain better chemical efficiency, better recycling efficiency, and improved separations. However, I believe it will be difficult to obtain quantum improvements in this cost category.

In the area of capital investment reduction, some recent examples of the introduction of new process technology include the use of structured packing in order to increase capacity in the columns with lower holdup. Another interesting area is reactive distillation, where two functions are combined into one unit operation instead of requiring two separate unit operations. Recently my research group has been performing research on modeling and control of reactive distillation. There have been a number of notable commercial successes with reactive distillation (TAME, MTBE, methyl acetate), but it is unclear how many other processes could benefit from reactive separations. The goal is to increase the yield over equilibrium by performing reaction and separation in the same vessel. Such cases are restricted to exothermic reactions and equilibrium-limited reactions, where the normal operating conditions for separation and reaction overlap. At UT Austin we are carrying out two experimental projects using reactive distillation for production of TAME and detergent alkylate. We are investigating challenging control problems that come about when separation and reaction are combined in the same vessel. Table 4 compares the effects of three typical disturbances for the two column types: feed-flow change, feed enthalpy change, and column pressure change. When using reactive distillation, new control problems may arise. For a feed flow change, the residence time changes in the system, which in turn changes the reaction characteristics. This must be dealt with through some sort

Disturbance	Distillation	Reactive Distillation
Feed Flow change	Effectively handled by manipulating variables ratioed to the feed rate	Change in residence time over catalysts must be treated
Feed enthalpy change	May significantly alter internal L/V for low reflux columns	Low reflux ratios employed under kinetic control
Column pressure change	Changes relative volatility, usually with negligible effect	Pressure directly affects temperature profile in reaction zone

Table 4. Comparison of the Effect of Disturbances on Conventional Distillation vs. Reactive Distillation

of advanced model-based control strategy. Pressure changes are usually not too difficult to handle in a conventional column, but in a reactive distillation column the temperature profile may change markedly. The above examples illustrate new process technology will require new operating strategies and that the resulting plants may be more difficult to control.

The batch industry is overlooked in traditional chemical engineering courses. Most papers and textbooks typically use examples of continuous processes, but smaller-sized batch plants actually account for about half of the production tonnage in the United States [2]. One of the areas in batch scheduling that will receive more attention in the future is the use of just-in-time production to reduce the cost of storage and inventory. If one can keep inventory at a minimum, these plants will be much more agile carrying out process changes and changing from one product slate to another. In order to reduce costs, it is desirable to manufacture products with a short cycle time.   This goal will require an increased emphasis on modeling and control in batch processing.

Plant Operations and Information Technology

While the design of new facilities will continue to be the purview of process engineers, the next 20 years will undoubtedly see a greater emphasis in the use of information technology in plant operations [4]. A new stage in the evolution of plant information and control architectures is now emerging. The last 20 years of progress in computer control has been spurred by acceptance across a wide spectrum of vendors of the distributed control hub system for process control, which was pioneered during the 1970s by Honeywell. A distributed control system (DCS) employs a hierarchy of computers. A single microcomputer controls 8 to 16 individual control loops, and more detailed calculations are performed using workstations, which receive information from the lower-level devices. In this scheme set points, often determined by real-time optimization, are sent from the higher level computers to the lower level microprocessors. Now with the focus on enterprise integration, some automation vendors are implementing Windows NT as the new solution for process control, utilizing personal computers in a client-server architecture rather than the hub-centric approach used for the past 20 years. This promotes an open application environment (open control system) and makes accessible the wide variety of PC object-oriented software tools that are now available.

The demand for smart field devices is rising rapidly. It is desirable to be able to query a remote instrument and determine if the instrument is functioning properly. A digital-based instrument (rather than analog) has the key advantage that signals can be transmitted digitally (even by wireless) without the normal degradation experienced with analog instruments. In addition, smart instruments have the ability to perform self-calibration and fault detection/diagnosis. Smart valves include PID control resident in the instrument, which can permit the central computers to do more advanced process control and information management. It is projected that installations of smart instruments can reduce instrumentation costs by up to 30% over conventional approaches. There has been much recent activity in defining standards for the digital, multidrop (connection) communications protocol between sensors, actuators, and controllers. In the U.S. the concept is called fieldbus control, and vendors and users have been working together to develop and test interoperability standards via several commercial implementations.

When data become readily available at a central point, it will be easier to apply advanced advisory systems (e.g., expert systems) to monitor the plant for performance as well as detect and diagnose faults. Recent efforts have built on the traditional single variable SPC approach, extending it to multivariable problems (many process variables and sensors) using multivariate statistics and such tools as principal component analysis. These techniques can be used for sensor validation to determine if a given sensor has failed or exhibits bias, drift, or lack of precision. Maintenance of the chemical plant will be integrated with operational activities, using sophisticated tools such as data mining to improve reliability. Maintenance data bases will contain full knowledge of all equipment, and knowledge-based computers will monitor routine and preventive repairs, utilizing expert systems to prevent failure through the proper level of maintenance.

In the area of process modeling industrial groups are beginning to examine whether it is possible to achieve a seamless transition between models used for design and simulation and models used for control. The CAPE-OPEN industrial consortium in Europe and other groups in the U.S. are working towards an open architecture for commercial simulators to achieve "plug and play" using company-specific libraries such as physical property packages. The extension of these steady-state flowsheet simulators to handle dynamic cases is now becoming an active area (e.g., linking Aspenplus to Speedup). The goal is to have models for real-time control that run at 50 to 500 times real-time, but this will require increased computational efficiency and perhaps application of parallel computing. Models for any use should be derivable from a single source, and dynamic models should be an extension of steady-state equations. Models should be robust and insensitive to starting conditions and should match the full operating range of the plant. Standard data exchange is needed so that models in the library can come from different sources.

A new generation of model-based control theory has emerged that is tailored to the successful operation of modern plants. These advanced algorithms include model predictive control, robust control, and adaptive control, where a mathematical model is explicit in developing a control strategy. The success of model predictive control (MPC) in solving large multivariable industrial control problems is impressive [5], perhaps even reaching the status of a "killer application". Model predictive control of units with as many as 10 inputs and 10 outputs is already established in industrial practice. Computing power is not causing a critical bottleneck in process control, but larger MPC implementations and faster sample rates will probably accompany faster computing. Improved algorithms could easily have more impact than the improved hardware for the next several years. MPC will appear at the lowest level in the DCS, which will reduce the number of PID loops implemented.

Recent announcements by software vendors indicate that the combination of process simulation, optimization, and control into one software package will be a near-term reality, at least if some corporate mergers and acquisitions are any indication, Aspentech's acquisition of Dynamic Matrix Control Corporation, Setpoint, Inc., and Neuralware will provide the ability to offer integrated technology with a set of consistent models across R&D, engineering, and production stages, with increased emphasis on rigorous dynamic models and the best control solutions. Similarly, Shell Oil Company and Simulation Sciences have developed a new modeling software system called rigorous on-line modeling and equation-based optimization (ROMEO). Simulation Sciences was recently acquired by Siebe, who also owns Foxboro, historically one of the stronger process control vendors. As a result of these mergers, software users will be able to optimize plant-wide operations using real-time data and current economic objectives. The equation-based approach is expected to be faster than the sequential-modular (unit operation) methodology. The software can determine the location and cause of operating problems and provides a unified framework for data reconciliation and parameter estimation in real-time.

Further movement towards the Computer-Integrated Manufacturing (CIM) paradigm is expected. CIM is defined as a unified network of computer hardware and software systems that combines the business and process functions (such as administration, economic analysis, scheduling, design, control, operations, etc.). This includes interactions among suppliers, multiple plant sites, distribution sites, transportation networks, and customers. Operations will be guided by complete information throughout the supply chain, i.e., integration of sales, marketing, manufacturing, supply, and R&D data where data and information flow in a seamless fashion along the whole supply chain. CIM provides general access to a common data base and produces reports for managers, engineers, and operations so that optimum decisions can be made and executed in a timely and efficient manner. CIM is recognized as an important tool for improving the competitiveness of the U.S. process industries, but CIM is not yet implemented in a significant number of plants. Cooperation among computer vendors is required to develop a satisfactory computer/communication/software system.

Supply chain management poses difficult decision-making problems because of the wide ranging temporal and geographical scales, along with a high level of uncertainty because of changing market factors and plant availability. A successful package of tools must anticipate customer requirements, commit to customer orders, procure new materials, allocate production capacity, schedule production, and schedule delivery. In today’s manufacturing environment, most of these decisions are made in management “silos”, i.e., marketing, procurement, manufacturing, distribution, shipping, and sales all operate fairly independently. Successful supply chain management will require breaking down or re-engineering these silos. A company that is “able to promise” to its customer base will have a competitive advantage in the future. Technology tools required to achieve the “able to promise” state include forecasting, optimization, simulation, and expert systems. Manufacturing operations will respond to customer demand that comes either by pull or by make-to-order. This demand drives scheduling, raw material supply, distribution, deployment of manufacturing resources, and production. The system will operate automatically without manual intervention; logic and expert systems will make the routine decisions.

In the factory of the future, the industrial environment where process control is carried out will be different than it is today. In fact, some forward-thinking companies believe that the operator in the factory of the future may need to be an engineer as done in Europe, with economic and safety responsibilities comparable to those of an airline pilot. Because of greater integration of the plant equipment, tighter quality specification, and more emphasis on maximum profitability while maintaining safe operating conditions, the importance of process control will increase. Very sophisticated computer-based tools will be at the disposal of plant personnel. Controllers will be self-tuning, operating conditions will be optimized frequently, fault detection algorithms will deal with abnormal events, total plant control will be implemented using a hierarchical (distributed) multivariable strategy, and expert systems will help the plant engineer make intelligent decisions (those he or she can be trusted to make).

Plant data will be analyzed continuously, reconciled using material and energy balances and nonlinear programming, and unmeasured variables will be reconstructed using parameter estimation techniques (soft sensors). Digital instrumentation will be more reliable, will be self-calibrating, and composition measurements which were heretofore not available will be measured on-line. There are many industrial plants that have already incorporated several of these ideas, but no plant has reached the highest level of sophistication over the total spectrum of control activities. Figure 2

[6] illustrates a possible hierarchical CIM structure that could be used in merging business optimization with plant and process operations and control. Each layer will have different models and time scales and includes checking the model against data obtained by the computer systems. Consistent, robust models serve as the central repository of process knowledge. This will require advances in model building, which is a major obstacle because of the level of expertise required to formulate and use mathematical models.

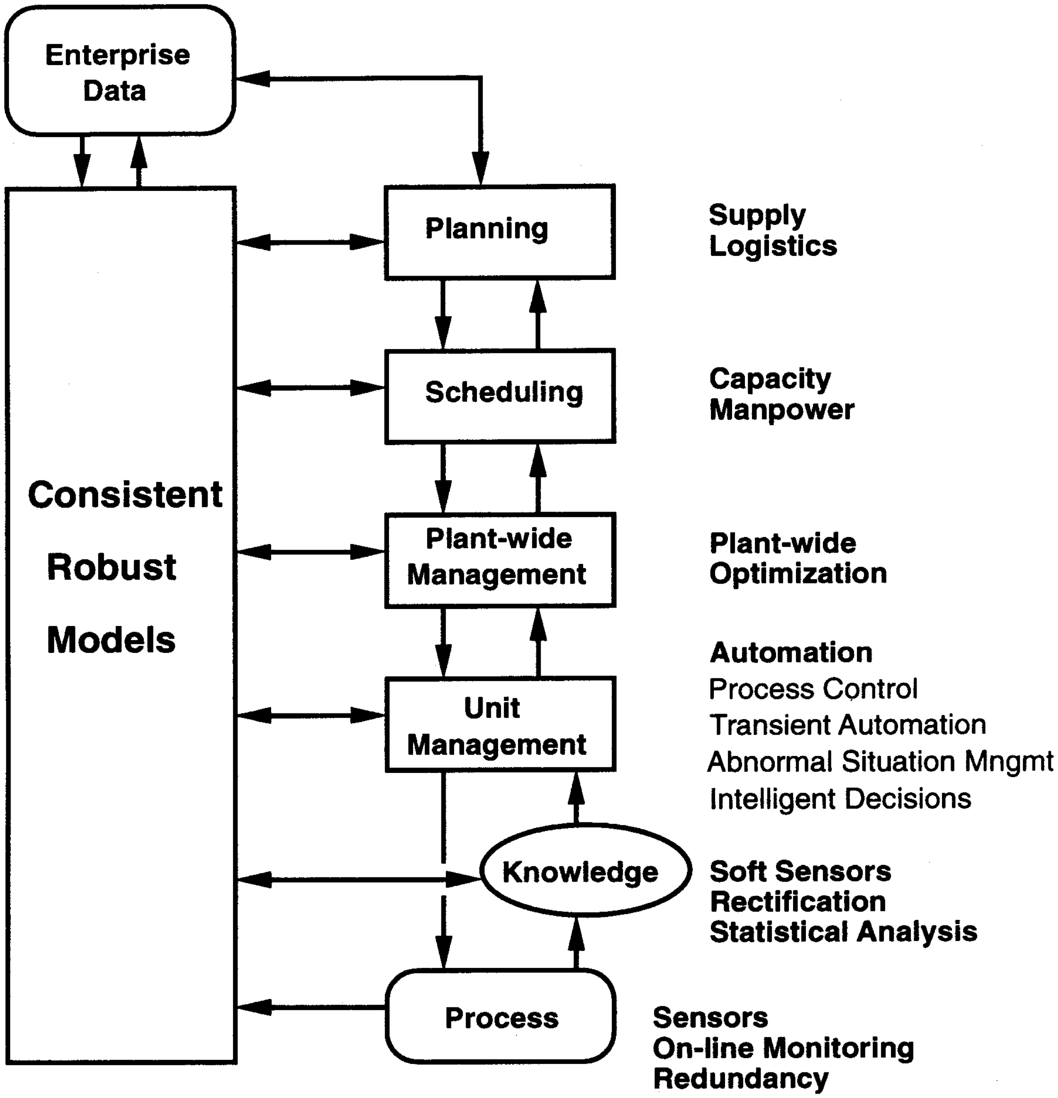

Figure 2. Model-based Computer-Integrated Manufacturing

Future batch plants will respond to schedules to meet production requirements using raw materials made available in parallel with the plant's response. The plant also will inform the plant computer system of the status and availability of equipment, people, materials, maintenance needs, and other elements needed to support automated scheduling. Both continuous and batch processes will have fully automated handling systems for raw materials, package components, and finished products. Robotics will be used extensively to minimize manual labor. This activity, combined with complete process automation, will minimize the need for manual intervention.

At the planning and scheduling level, multi-period linear programming tools capable of handling large scale systems have been used since the 1970s, especially in the petroleum/petrochemical sector. Real-time, plant-wide optimization applications using steady state process models are stimulating the use of nonlinear programming tools. The methodology for scheduling of multipurpose batch and continuous production facilities has been under investigation for over 20 years originally using rule-based and heuristic randomized search methods and more recently mixed integer programming methods.

An excellent video on how real-time decisions in manufacturing will be made in the 21st Century was made by E.I. Dupont de Nemours and Digital Equipment Corporation in 1991 [7]. Although this video is almost nine years old, it captures many of the elements of 21st Century process engineering discussed above and illustrates the effect of globalization on future manufacturing issues. It also demonstates how modeling and simulation can assist in dealing with issues of off-spec products, improved control strategies, and abnormal situation management.

The growth in complexity of the automated plant environment can be mitigated through the use of AI (artificial intelligence) tools to assist the operators and engineers. Thirty one years ago Stanley Kubrick presented the indelible image of HAL, the thinking computer, in the film, “2001. A Space Odyssey”. While there have been significant improvements in AI technology since 1970 (although modest compared to some previous claims), entering the millenium has inspired new predictions about future machine intelligence. In Kurzweil’s new book [8], he contends that with the dramatic advances in computing power, machines will surpass humans in intelligence at some point in the next century, threatening the human race as a species. Human cognition will be augmented by downloading thoughts and memories into computers, moving to some form of machine consciousness. Indicative of this trend, in 1998 the IBM Deep Blue chess computer defeated one of the best chess players in the world (Gary Kasparov). Such ideas are being hotly debated now, and it will be interesting to see whether this latest group of futurists are more accurate than predictions made thirty years ago.

Educational Implications of Advances in Computer Technology

There is no doubt that the revolution in computing and information technology during the past 40 years has changed the industrial world and process engineering. In contrast, the typical engineering educator, rather than being on the cutting edge of those developments, has been slow to incorporate new computer-based ideas in curriculum, teaching methodologies, and educational materials. With a few notable exceptions, computing and information technologies have not had a major impact on the chemical engineering canon. At most institutions, thermodynamics and transport phenomena are not taught any differently than they were 30 years ago. It is apparent that in the eyes of a large number of faculty the investment made by students in learning computer languages and programming does not yield any discernible advantage in the training of chemical engineers.

The questions of how extensively computers should be used and which computing skills should be taught in the undergraduate chemical engineering curriculum are difficult to answer for several reasons:

1. There is no generally agreed upon ‘core’ set of computing skills or professional software tools necessary for being a productive engineer, either in academia or in industry.
2. Providing and maintaining a state-of-the-art facility for engineering computation is expensive, in terms of both capital and human resources.
3. Development of high quality computer-based lessons is quite costly in terms of faculty and staff time, and faculty are challenged to stay up-to-date.

Recent improvements in professional software may help faculty stay up-to-date. A so-called meta-computing approach uses software modules, does not require student or faculty knowledge of FORTRAN, and is interactive via a graphical user interface (GUI). MATLAB is a good example of the meta-computing approach. Automatic generation of html statements is now possible with Microsoft WORD, and incorporation of audio and video via the world wide web will become quite straightforward in the future, making distance learning to the desktop a real possibility.

Educational institutions and their departments must shoulder the burden of lifecycle planning for hardware and software, in order to keep up-to-date computer tools in the hands of faculty, staff and students. This is different from the approach currently taken at many universities, where faculty and departments must fend for themselves due to inconsistent funding models for new technology. Information technology costs are approaching 10 to 20% of total costs in corporations today, and university cost structures are expected to follow suit. Training of faculty must be given a high priority and encouraged as part of faculty development programs. Release time for faculty to develop content for technology – enhanced learning also must be provided. University administrators must adjust the faculty reward system so that there are incentives for faculty to introduce technology in their teaching. The world wide web gives faculty a new publishing vehicle for their lecture material, and eventually for research publications in peer-reviewed on-line journals. These topics deserve considerable discussion, but that is the subject of another lecture [9].

Acknowledgment

I would like to thank Phillips Petroleum Company for their continuing support for the Phillips Lecture, which has become a nationally prominent forum for ideas on chemical engineering education. I started receiving the Phillips Lecture pamphlets about 15 years ago, and have looked forward to reading them each year since that time. Being selected as the 1999 Lecturer has special significance for me as I am a native Oklahoman from Bartlesville (or "Bartian") and in fact worked for Phillips Petroleum one summer while an undergraduate. I also have a connection to Oklahoma State University, in that my three brothers were students there.

References

1. Naisbitt, J. *Megatrends*, Warner Books , New York, 1982.

2. Keller, G.E., and Bryan, P.F. "Process Engineering Challenges of the 21st Century," *Chem. Engr. Prog.*, in press (1999).

3. Trainham, J.A., "Benefits of Fundamental Modeling and the Need for Improved Simulation Tools and Modeling Environment", Internal Report, E.I. Dupont de Nemours, Wilmington, DE, July, 1996.

4. Vision 2020, http://www.chem.purdue.edu/v2020, Council for Chemical Research website.

5. Qin, S.J. and T.A. Badgwell, "An Overview of Industrial Model Predictive Control Technology", *Chemical Process Control V Conference*, AIChE Symposium Series, 93, no. 316, p. 232-256 (1997).

6. Edgar, T.F., Reklaitis, G.V., and Dixon, D.A. Vision 2020: "Computational Needs of the Chemical Industry", *Workshop on Impact of Advances in Computing and Communications Technologies on Chemical Science and Technology*, National Academy Press, Washington, D.C., 1999.

7. "The Edge", video developed by E.I. Dupont de Nemours and Digital Equipment Corporation, (1991) provided by Robert Cox of Dupont

8. Kurzweil, R. *The Age of Spiritual Machines: When Computers Exceed Human Intelligence*, Viking Press, New York, 1999.

9. Edgar, T.F. “Information Technology in Chemical Engineering Education: Evolution or Revolution”, Chemical Academy Lecture, University of Missouri, Rolla, MO, April, 1999.