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Computer Information Technology in Chemical Engineering Education

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The use of computers in the chemical and process industries has exploded in the last two decades. Computers are ubiquitous in business and education. Chemical engineering principles remain largely the same, though, and this paper describes how computers have impacted, or not impacted, the education of chemical engineers.

I. Computer Aids to Calculation.

Computers can be used to aid traditional learning, but using modern tools. The core chemical engineering curriculum has not changed much in the last twenty years: mass and energy balances, thermodynamics, fluid flow, heat transfer, mass transfer, kinetics and reactor design, control, and design, with a goodly amount of laboratory work thrown in. Computers are used in some of these courses, by some professors, but not all. The reason is given by Tom Edgars, Associate Vice President of Academic Computing at the University of Texas, and former President of the American Institute of Chemical Engineers, "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." [1]

Despite this negative viewpoint by some faculty, computers are used routinely in some chemical engineering courses. For example, at the 1997 Summer School for Chemical Engineering Faculty, Michael B. Cutlip from the University of Connecticut organized a session showing how various packages could be used to solve a set of ten standard chemical engineering problems. Some of them are:

Solving a mass balance on a separation train (simultaneous linear equations)

Fitting data to a curve, including nonlinear regression
Solving reaction equilibria (simultaneous nonlinear equations)
Solving for unsteady heat transfer of a lumped parameter system (ordinary differential equations as initial value problems)
Solving diffusion with reaction in a slab (ordinary differential equations as boundary value problems)
Solving gas phase reaction in catalytic reactor (simultaneous differential and nonlinear algebraic equations)
Solving the dynamics and control of a heated tank (stiff ordinary differential equations)

The solutions to these problems are available on CD-ROM and on the internet [2]. Mass transfer courses lend themselves to the use of computer, with examples like ChemSep for multicomponent separations and MultibatchDS for batch distillation [2]. Anklam, Prud'homme and the author [3] use numerical analysis to analyze laboratory chromatographic results in the undergraduate laboratory.

Computers are more likely to be used in education, though, if they professor doesn't have to babysit the users. Thus, commercial packages are becoming more pervasive. A recent article published by the AIChE describes how to pick the right software, from among Maple, Mathcad, Mathematica, Matlab, and TK Solver [4]. The chemical engineering problems described above are all solved with the first four of these, plus POLYMATH [2] and Excel [5]. Matlab is described as the best all-around mathematical tool for design and analysis for engineers working in the field of process control or performing data analysis, or when using numerical methods. For engineering calculations, Matcad, Matlab, and TK Solver are "obvious choices" while for research in mathematical analysis Maple and Mathematica are preferred.

II. Learning New Things Made Possible by the New Tools.

Computers began to make a big difference in education even as early as the mid-1970s. The process simulation program was FLOWTRAN, which was made available by Monsanto to Universities free of charge. This allowed large scale simulations involving interacting units with recycles - problems that had required weeks to solve previously. It also permitted more realistic choices of thermodynamics models, including thermodynamics appropriate to polar, non-ideal molecules. Thus, students are able to see interactions among units, and approach the problem more from a systems viewpoint, with realistic results, rather than using unrealistic assumptions to reduce the problem to a manageable level.

Today it is possible to use computational fluid dynamics programs to solve the Navier-Stokes equations, plus energy and concentration equations, in two- and three-dimensional cases, possibly including turbulent flow are particulate transport [6]. The program PDE TOOLBOX that is an add-on to Matlab, provides finite element solutions to single elliptic equations. This program is easy to use, and it has been used in heat transfer courses to demonstrate two-dimensional effects in heat transfer. Students are intrigued by the colorful displays of the solution, and if they can be taught to check the results, and obtain useful information from the solutions, these programs allow students to solve problems without making assumptions that have been justified in the past based not on their reasonableness but on the fact that they simplified the problem enough that it could be solved.

III. Multimedia Tools - Learning in a New Way.

As computing power increases faculty are developing entirely new ways to learn chemical engineering. For example, Purdue University has developed simulations of industrial processes for use in senior laboratory courses [2]. In addition, interactive games are being used to pique students' interest [2], and a visual encyclopedia of chemical engineering equipment has been prepared [2]. A suite of interactive computer modules has been developed at the University of Michigan to teach material and energy balances, fluids and transport, separations, and chemical reaction kinetics [2]. These modules have been tested over several years at several Universities, and provide an interesting approach to learning by using common, everyday examples that can illustrate chemical engineering principles.

The widespread use of the internet also provides a new mechanism of communication which chemical engineering students need to learn, and which helps them learn as well. The author has had students prepare web lessons about the subjects treated in class. Examples are: converting oil to polyethylene garbage bags, modeling microchemical reactors, and fluidized beds [7]. The way these ideas are weaved into a course to allow much project and group work is described in papers given at meetings of the American Society of Engineering Education [7].

Information technology does allow better distance learning courses. While ε lecture may be broadcast by satellite, the class materials can easily be transmitted as attachments to electronic mail or as Adobe Acrobat pdf files obtained via ftp. Even more effective are class materials that involve interaction, delivered via the internet or CD-ROM. Finlayson, in his Phillips lecture [7], describes several methods oı instruction: distance learning via TV transmitted over satellites, satellite campuses, lectures on demand, and the internet, multimedia, and CD-ROM. Each of these was evaluated based on cost comparisons as well as learning theories of retention. Technology, though, has far outstripped what was available in 1996. Now possibilities include wireless, handheld devices, voice recognition, and high-speed video transmission [8].

IV. Industrial Activity and University Research that Drives Information Technology in Chemical Engineering.

A forecast of future advances in process modeling, control, instrumentation, and optimization is part of the report *Technology Vision 2020: Report of the U.S. Chemical Industry* [9]. A summary of the computational needs is provided in the workshop report of the Chemical Sciences Roundtable [10]. Most process engineering research has devolved into four areas: process design, structure-property relationships, process control, and process operations. It would be desirable if the following could be predicted: biological activity from chemical structure, environmental fate from chemical structure, efficient catalysts, efficient processes from an understanding of microscopic molecular behavior, material with a given set of target properties. The technologies needed to do this include high-performance, scalable, and portable computer codes for parallel computer architectures, improved problem-solving environments to make computational tools more accessible, improved database and data-analysis technologies, computer-aided synthesis methods focusing on materials, and computer architectures, operating systems, and networks.

V. Conclusion.

The use of technology in chemical engineering education requires the followin components, as described by Doherty, *et al.* [6]. "The faculty must have tł enthusiasm and release time to change from the traditional lecture format. The must be willing to adapt during class to student discoveries and interests. Software tools must be familiar to the faculty and teaching staff, *before* the class starts. Examples must be developed and tested in the working environment *before* classes. A minimum amount of professional staff time is needed to maintain the computer systems, and for faculty/TA training and support."

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