THE DEVELOPMENT OF CHEMICAL ENGINEERING DESIGN COMPUTER PROGRAMS.

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Summary. New developments in process and plant design computer programs is described, particularly process minimization, intensification and integration. The trend of this development is leading to compact, safe, energy efficient, environment-friendly, flexible processes and plants. However the teaching of chemical engineering will have to undergo some essential revision; so the curriculum of chemical engineering education should be adjusted to the future needs of the chemicals production and construction companies. In this way the faculty members are encouraged to work together with these companies to investigate new development in process and plant design, eventually by using mathematical programming and optimization analysis with the help of adequate computer programs.

1. Background information.

Michael E. Lesley wrote in 1982 [1] that at that time software houses such as CHEMSHARE were leasing to large companies their process simulation programs in mainframe computers at the amount of a hundred thousands of dollars a year. Meanwhile small software houses such as COADE were trying to introduce into the market the process simulation program " MICROCHESS" for PC's at the one-time cost of $ 6,500.

But this PC program has been improved very fast just at the same speed as the development of the PC's. The software house COADE separated into two firms, namely Chemstations, Inc. and COADE, Inc. Chemstations specialized in chemical engineering programs such as Chemcad, costing more than $ 18,000 and other additional programs linking with Chemcad, and COADE continued with their mechanical engineering design programs such as CAESAR-II (Pipe stress analysis), Pressure Vessel and other programs.

In the beginning other software houses such as Chemshare, Hysis, Prosim, Aspen and others came with chemical process simulation programs for mainframe or mini-computers, but later on they all converted their programs into PC format. All these software houses have developed their chemical process simulation programs with new features such as: cost estimation, equipment design, sensitivity analysis, optimization, pinch analysis and others, not including additional engineering programs such as heat-exchanger -, reactor -, batch distillation -, and dynamic column design, etc.

In addition to the standard requirements for comprehensive thermodynamics and unit operations, such a process simulation tool should have the following major characteristics:

1. It should run in both steady state and dynamics mode.
2. It should have a good system for economic analysis which includes equipment sizing, plant cost estimation, and present value analysis of cash flows.
3. It should be able to include the effects of equipment sizes and geometry on the simulation by accounting for heat and mass transfer resistances and pressure drops.
4. It should have optimization and case study facilities.
5. It should easily incorporate plant and experimental data.
6. It should be easily customizable
7. It should be able to document not only the results of calculations, but also the history of the design development process itself.
8. It should be able to communicate with other software.

Nowadays all the modern commercially available chemical engineering design programs should be capable to fulfill such characteristics.

2. New developments in process simulation and design programs.

2.1. The New Paradigm.

Today increasing worldwide competition is mandating major changes in the way plants are to be designed. As a result, we are witnessing dramatic new developments that go beyond “traditional” chemical engineering. New equipment technologies and novel techniques are emerging that potentially could transform our concept of chemical plants and process engineering, leading to compact, safe, energy efficient, environment-friendly, flexible processes and plants.

Keller and Bryant [2], in their article on the new directions of process engineering, identified seven themes that will affect the design of process plants over the following years. These are:

1. Raw material cost reduction.
2. Capital investment reduction.
3. Energy use reduction.
4. Increased process flexibility and inventory reduction.
5. Greater emphasis on process safety.
6. Increased attention to quality.
7. Better environmental performance

There is a powerful extension of the use of process design that until today has been little exploited. This involved the intimate intermingling of experimental research and development with process modeling and design. The new paradigm involves the initiation of serious process design right at the beginning of a project. In fact, following the initial eureka, the first activity should be the development of a flow sheet with material and energy balances, a thermodynamics package, very rough equipment sizing, and a simple economic model. Many guesses and approximations will have to be made in this early flow sheet, but the purpose of this activity is to focus the experimental program as quickly as possible on the critical technical and economic questions regarding the process. Massey gave in his paper [3] a sample (Azeotropic distillation of ethanol and n-pentane) of such application by using a new version of a sophisticated process simulation computer program.

.2.2. Process Minimization.

Dennis C. Hendershot recommended [4] minimization in process design in order to lessen the consequences of potential mishaps via reducing hazardous inventories, reactor size, and even pipe diameters. But also reducing the quantity of a hazardous material or energy through process minimization is one important way of increasing the inherent safety of a CPI process. For instance, modern nitration plants use small continuous stirred-tank reactors that provide intense mixing and large heat-transfer areas or jet reactors to deliver the intense mixing and rapid contacting of reactants.

Another example is the polymerization process of a continuous-loop reactor that is more compact, efficient and inherently safer than traditional batch equipment. Conducting one or more unit operations in a single piece of equipment is another approach to process minimization.

Reactive distillation is a good example. For instance a traditional route for making methyl acetate that uses a stirred tank reactor, eight distillation columns, and an extraction column can be replaced by a new reactive distillation process that uses one such column and two additional distillation columns, significantly lowering the inventory and number of major vessels.

Process minimization will dramatically reduce the size of equipment required to carry out various operations as to be a key step in reaching this future state of the CPI.

2.3. Process Intensification.

The term for the evolving techniques and methods that will be used to meet these more stringent requirements is “Process Intensification”. In 1995, while opening the First International Conference on Process Intensification in the Chemical Industry, Ramshaw, one of the pioneers in this field, defined process intensification as a strategy for making dramatic reductions in the size of a chemical plant so as to reach a given production objective. These reductions can come from shrinking the size of individual pieces of equipment to reducing the “size” of the process by reducing the number of pieces of equipment required. Ramshaw speaks about volume reduction factor on the order of 100, but even a reduction factor of two would require major changes in plants and equipment.

Process intensification concerns only engineering methods and equipment. So, for instance, development of a new chemical route or a change in composition of a catalyst, no matter how dramatic the improvements they bring to existing technology, do not qualify as process intensification.

André I. Stankiewicz and Jacob A. Moulijn [5] offer the following definition: “Process intensification consists of the development of novel apparatuses and techniques that, compared to those commonly used today, are expected to bring **dramatic** improvements in manufacturing and processing, substantially decreasing equipment-size/production-capacity ratio, energy consumption, or waste production, and ultimately resulting in cheaper, sustainable technologies. Or, to put this in a shorter form: any chemical engineering development that leads to a substantially smaller, cleaner, and more energy-efficient technology is process intensification! The whole field of process intensification generally can be divided into two areas:

Process-intensifying equipment, such as novel reactors, and intensive mixing, heat-transfer and mass-transfer devices and

Process-intensifying methods, such as new or hybrid separations, integration of reaction and separation, heat exchange, or phase transition (in so-called multifunctional reactors), techniques using alternative energy sources (light, ultrasound, etc.), and new process-control methods (like intentional unsteady-state operation).

The new paradigm mandates the initiation of serious process design right at the beginning of a project; that is, right from the initial ideas and before the laboratory research begins. In fact, following the initial "idea", the first activity should be the development of a process flow sheet with material and energy balances, a thermodynamics package, rough equipment sizing, and a simple economic model. Many guesses and approximations will have to be made at this early stage, but the purpose of this activity is to focus the experimental program as quickly as possible on the critical technical and economic questions regarding the process

2.4. Process Integration.

As mentioned before, improved product quality is one of the themes driving these changes, and improved process control will be a key issue for achieving quality goals. In addition, the process changes driven by several of the other themes will also require better process control technologies. For example, the effort to reduce investment will cause equipment to be downsized to the maximum possible extent, eliminating much of the extra volume in process equipment. Currently, this additional volume contributes to smoother plant operations and provides safety margins for reducing off spec production. Likewise, surge tanks will disappear. The desire to reduce the amount of hazardous material present and to build speed and flexibility into the plant will also argue for reducing surge capacities. These changes will make processes more prone to going out of control. Therefore, improvements in the design of process control systems will become increasingly necessary to prevent off spec product.

The above trends will clearly demand greater functionality and tighter integration of computerized process design tools. In order to meet the demands of this more integrated and fast moving engineering paradigm, the simulation tool itself will need to be more integrated and comprehensive; and it must do this in a way that will make it easy for a wider range of people to use and understand it

According to Nick Hallale [6] in the past, the major research in process design has been placed on the analysis, or simulation of process. The synthesis of processes or process integration has, in comparison, received little attention. However, this is all changing. Until recently, process integration was virtually synonymous with pinch analysis and energy integration. However, over the past few years, there have been two significant trends that change this picture.

First, a wider range of solution techniques is now used. Rather than using only thermodynamics, or pinch methods, the advantages of **mathematical programming and optimization** have been combined. The insights from thermodynamics have been retained and combined with the power of mathematical methods for data handling, optimization and automatic design. The approach used as far as possible is to develop a deep understanding of the physical principles underlying problems, and only then to develop practical methodologies that employ the necessary mathematics. The power of these methods is undeniable, but they are virtually impossible to apply without the use of computer software.

3. The trend of Chemical Engineering Education.

Stankiewicz. and Moulijn [5 - page 34] have the opinion that the teaching of chemical engineering also will have to undergo some essential revision. Firstly, future chemical engineers will have to be taught an integrated, task-oriented approach to plant design, unlike today's sequential, operation-oriented one. To achieve this goal, the education of future engineers must place much more stress on creative, no schematic thinking and not only confined to known types of equipment and methods. Secondly, future chemical engineers must gain a much deeper knowledge and understanding of process chemistry, because in the highly efficient chemical processes of the coming decade, chemistry and engineering will be meeting each other at the molecular level, not at the apparatus level as they do today. Thirdly, material engineering will play an essential role in the development of new chemical processes at the molecular level (engineering of catalyst) and therefore will become a much more important part of the chemical engineering curriculum.

Thomas F. Edgar said [7] 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 these developments, has been slow to incorporate new computer-based ideas into the curriculum, the teaching methodologies and educational materials. Computing and information technologies have not had a major impact on the chemical engineering canon. Thermodynamics and transport phenomena are not taught any differently than they were 30 years ago. But recently improvements in professional software programs may help faculty stay up-to-date.

To keep up-to-date computer tools in the hands of faculty, staff, and students, educational institutions and their department must adopt life cycle planning for hardware and software. In corporations today information technology costs are approaching 10-20 % of total costs, and university cost structure are expected to follow suit. Training must be given a high priority and encouraged as part of faculty development programs. The World Wide Web gives educators a new publishing vehicle for their lecture material.

4. Conclusion.

It can be concluded that during the last two decades the commercial process simulation programs on PC's have pushed aside these programs installed on mainframe or minicomputers. These programs have been very much developed at the same speed as the development of the PC. These days these programs are mostly used by construction and chemical production companies, however on a very slow speed also by universities. But because of competition between these companies new equipments and methods are developed, so that the chemical engineering curriculum at the universities soon becomes more and more obsolete from the new developments in process and plant design.

Some universities are starting already to cooperate with a group of production companies in order to investigate new developments in process intensification and integration using commercial available software programs. We hope that this trend will also be extended to the universities in the ASEAN countries.

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