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COMPUTER AIDED PROCESS ENGINEERING

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Computer Aided Process Engineering is one sector in the field of *Process Engineering* defining all what is process related and computer assisted. It starts from the molecular modelling and passes through computation of physical or chemical properties, mathematical modelling and simulation, computer control, optimization and integrated process design. It is very applied engineering and nowadays the name is redundant because there is no physically existent process or product in elaboration which is not helped by computer if it is to be considered in the light of sustainable development or to be valued on the market.

Key words: Computer Aided Process Engineering, Mathematical Modelling, Monitoring, Control, Optimization, Process Design, Data Mining, Artificial Intelligence, Bio Informatics, E-Learning.

1. THE EVOLUTION OF PROCESS ENGINEERING

The *Process Engineering (PE)* is the field of industrial manufacturing or processing of whatever is useful in the everyday life: production of potable water, pulp and paper, pharmaceutical drugs, polyethylene, cars, steel, sulphuric acid, petrochemicals; production of energy, solvents, dyes, anticorrosive coating, enzymes, pheromones, cement, textiles, food, beverages, waste processing and minimization etc. It covers also the field of bio engineering.

Every scientific discipline has its characteristic set of problems and systematic methods for obtaining their solutions - that is, its paradigm. The origins of *PE* are in 1888, when at Massachusetts Institute of Technology, started a Chemical Engineering program, as an option to the program of Chemistry. First chemical engineering paradigm is the unifying concept of *unit operations* proposed by Arthur D. Little in 1915. The concept became operational around 1920, just during the first petroleum crisis; other classical tools of chemical engineering analysis were introduced: studies of the material and energy balance of processes and fundamental thermodynamic studies of multi component systems. The second paradigm of the field is the engineering science movement, consisting in *phenomena in unit operations that are resolved at the molecular level-micro scale*, mechanistic models for these events, and mathematical models of processes. The third chemical engineering paradigm expresses that nowadays, a confluence of intellectual advances, technological challenges, and economic driving forces shape a *new model of what chemical engineering is* and what chemical or already named process engineers will do: serve industries whose *products are quickly superseded* in the marketplace by improved ones; serve industries that *compete on the basis of quality and product performance*; expertise in the manufacturing of *composite and structured materials* from large molecules; expertise in the manufacture of *high-performance and specialty materials*; expertise in designing *small-scale processes, batch processes*; use more complete models, better approximations, and large computers to solve problems rigorously; have multiple career changes. Academic research is also performed by multidisciplinary groups of principal investigators; research and education also include the micro scale. In all these fields, one can observe a new paradigm is occurring, that of the *computational scientist.*

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The forces behind this evolution are the explosion of new products and materials, the increased competition for the world market and globalization, society's increasing awareness of health risks and environmental impacts.

In 1987, the National Research Council of the United States of America issued the so called "Amundson" Report [1] which established the seven important directions in which the *PE* will develop in the XXI century:

- Biotechnology and Biomedicine;
- Electronic, Photonic & Recording Materials and Devices;
- Polymers, Ceramics and Composites;
- Processing of Energy and Natural Resources;
- Environmental Protection, Process Safety and Hazardous Waste Management;
- ***Computer-Assisted Process and Control Engineering;***
- Surfaces, Interfaces and Microstructures.

Thus, the foresighted "Amundson" Report envisioned the distinct field of what we consider unavoidable today, *Computer Aided Process Engineering (CAPE).* More recent, one important workshop [2] figuring out the advances in *Information Technology* described the changes in product engineering. The synergies in chemical enterprise and information technology initiated unprecedented growth in the capability and productivity.

2. COMPUTER AIDED PROCESS ENGINEERING

The development of *CAPE* found its way related closely to the development of the computing hardware and the related software tools. Thus, the main directions of *CAPE* are nowadays:

- Modeling and Simulation of Unit Processes
- Studies on Flexibility, Operability and Dynamics of Processes
- Model-Based Manufacturing and Control
- Concurrent Process Engineering
- Whole Process Synthesis & Integration

All these developments take into consideration the recent affirmation of *Sustainable Development.* Sustainable development was set on the agenda by the Brundtland Commission with the definition: "meeting the needs of the present without compromising the ability of future generations to meet their own needs". Figure 1 shows the consequences of this philosophy and the impact on *CAPE*.

It is obvious that a new approach supported by *CAPE* comes to be taken into consideration: optimization, process improvement, process system design with sustainable options.

Modelling and Simulation in *PE* refers to molecular modelling [3], thermodynamic systems equilibria [4], or macro systems modelling. One example is *Computer Aided Drug Design*, which is an important contributor in the discovery and development of new pharmaceuticals. Special molecules are modelled and then created to have properties in healing some specific diseases. To a large extent, the modelling and simulation of the bio–processes taking place in the tissues or in the cell, are becoming more and more popular in approaching. The hydrodynamics of the drugs circulation, the release of the active principles in the body, the mass and heat transfer and chemical processes in the human body are studied largely [5], creating the expectations that in some years (not more than 10) we shall be able to describe, calculate and predict with high accuracy the effect of the drug on a certain specific target in the human body.

In *Simulation and Computational Methods for Design and Operation*, the predictions based on modelling are good enough to obtain phase diagrams for real gases with accuracies exceeding experiments.

The *Macro Modelling* refers to the description of the steady state or dynamics of the industrial plants which allows the implementation of improvements either in current operation, or in the structure of the plant [6,7,8].

The *Studies on Flexibility, Operability and Dynamics of Processes* allow, through *Sensitivity and Controllability Analysis,* the best operation mode of the plant, identification of the most important parameters in the functioning of the plant. In the department of Chemical Engineering at the Faculty of

Chemistry and Chemical Engineering in Cluj-Napoca there have been several researches in this field of *Sensitivity and Controllability Analysis* [9,10,11].

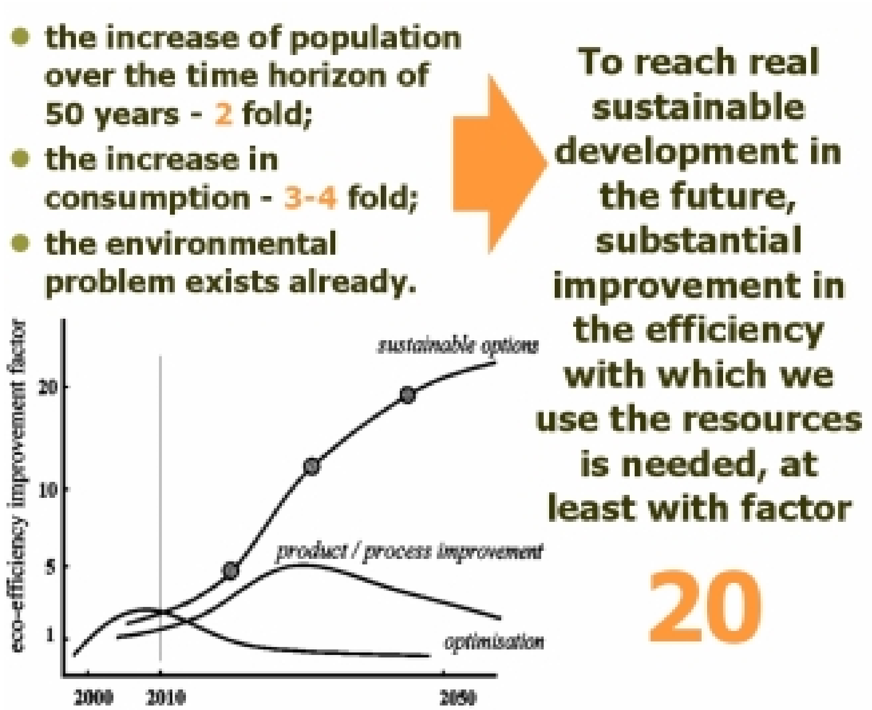

Figure 1. Sustainable development and the consequences on *CAPE*

The *classic control*, using feed back approach, is still in the best position in the process industry, regarding the number of applications, summing up around 80% [12,13]. There are also numerous new applications of the *classic control:* development of specific control systems for new technologies: new materials, bio technologies, de- pollution technologies; development of soft sensors [14] and better exploitation of data mining technologies in obtaining synthetic information [15]; increase in the safety of processes: detection, diagnosis and isolation of the faults –"fault-tolerant control". At the same time, *advanced control* is oriented towards the development of intelligent systems: expert systems, neural networks, fuzzy techniques, genetic and evolutionary algorithms [16-18]. Industrial data monitoring and processing are becoming more and more important in the management of the plants. An example is the monitoring and data processing system implemented at UPSOM Ocna Mures [15]. The main panel of the application, *System of Energy Management* is presented in the figure 2.

The system is working online since 1997, on a regular PC, in a very harsh industrial environment without major problems. The system is gathering the data from the different transducers positioned on the steam and other utilities production and consumption. It creates a historical archive of data on hourly, monthly annual basis, calculates the real thermal load of the steam fluxes and gives important information on the consumption in the different compartments of the soda ash factory. Based on this system, the users reported an energy saving estimated, in average, at 15%. The system uses the LabView programming environment

In more sophisticated situations, where the processes are either very sensitive or high energy consumers, one of the latest control approaches is the *Model Predictive Control*. (Figure 3). At each step, the manipulated variable is calculated in order to minimize the difference between the reference and the predicted output of the controlled plant. The prediction on a certain horizon of time is based on an *internal model* calculation.

Important researches in this field have been done in the Department of Chemical Engineering of "Babeş-Bolyai" University of Cluj-Napoca [19 - 22]. A good example is the research on *Fluid Catalytic Cracking Unit (FCCU)*, which started in 1992 at California Institute of Technology, USA, based on the request of Chevron Research and Development Department (Figure 4) and continued with the collaboration of SNC Petrom, Petrobrazi Refinery. The request of Chevron was to model and simulate another catalyst circulation and an improved control scheme , with the scope of stabilizing the process.

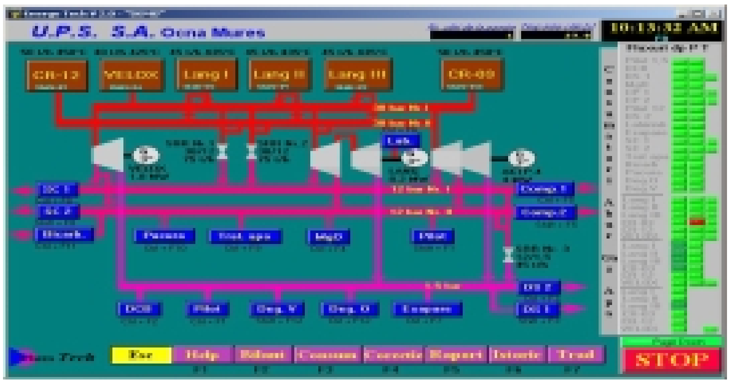

Figure 2. Main panel of the Energy Management System at Bega UPSOM thermo power station

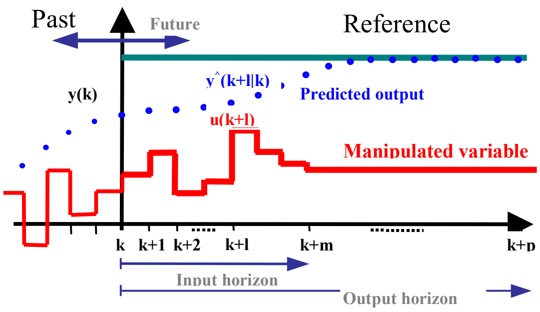

Figure 3. Model Predictive Control philosophy.

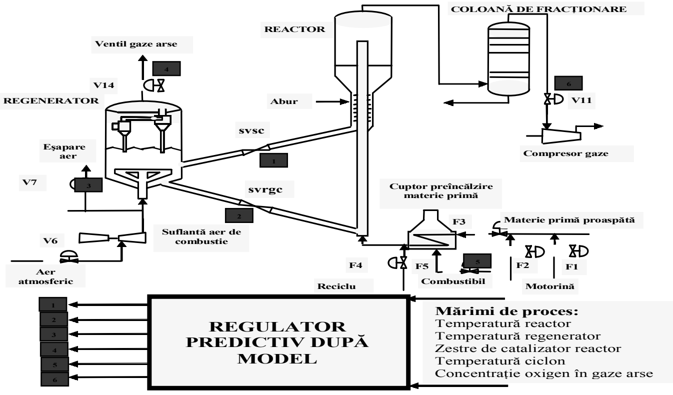

Figure 4. Model Predictive Control of FCCU

The example of this approach is very interesting because at stake was an investment of 40 million USD and the company wanted to know what results could be expected from the modifications. The results of the work [23] showed that a significant improvement of the stability of the process could be reached only through a modified procedure of operation and not through the important financial investment.

The research continued with the study of *Predictive Control* of another type of *FCCU* [24] working at the refinery Brazi, in Romania. Nowadays the *FCCU* plant in the OMV company Brazi refinery, is computer controlled and the basic control algorithms used are from the *model based* class. The control is hierarchical at three levels: equipment, plant and refinery, the last level having an economic optimization objective.

Other orientations of *CAPE* are in the field of *Process Optimization and Synthesis:* mathematical modeling and simulation of chemical processes using the integrated simulation and design software packages *ChemCAD, Aspen, Hysys, Pro/II, Matlab*; validation studies of mathematical models, retrofit, energy consumption reduction and optimization of chemical plants [25,26,27].

The last issue I would like to present in this paper on *CAPE,* is the *e-learning* or *CAPE education.* Nowadays we are speaking a lot about *sharing education through internet*. *E-learning* covers many aspects from *e-library access* to *remote location laboratories* [28,29]. Figure 5 sketches the organization of such a laboratory. The laboratory is computer monitored and controlled. It can be supervised through video cameras and microphones, the data, image and sound being transmitted to the remote location through *Data-Voice LAN* and farther, through Internet, using a *TCP/IP* protocol. From the remote location it is possible to measure parameters, to operate the pilot plant manually or automatically. In this way, the access to expensive equipment is facilitated, creating a virtual *Multiple User Laboratory*.

All the software allowing the communication between the two locations was developed in the Department of Chemical Engineering of "Babeş-Bolyai" University.

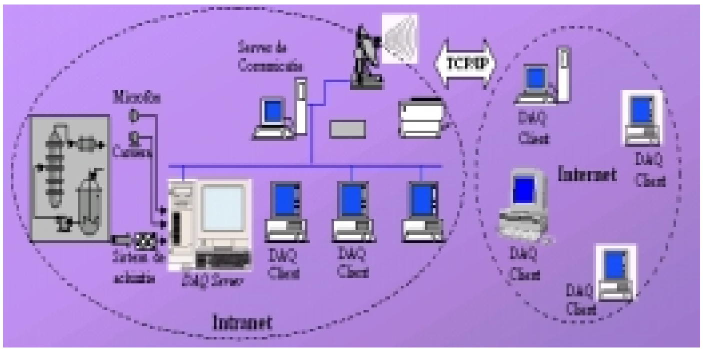

Figure 5. Remote control laboratory

3. CONCLUSIONS

CAPE is nowadays recognized as a special branch of *Process Engineering*. The *European Federation of Chemical Engineering* has a special *CAPE Working Party* which debates the developments of this chapter of *Process Engineering*. As it could be observed from the paper, very much of the *CAPE* activity can be identified as belonging to other fields of activity: *Control Engineering*, *Biochemical Engineering, Medicine, Information Technology, Environmental Engineering, Pharmaceutical Engineering, Chemistry and Chemical Engineering*. In fact, *CAPE* is a transdisciplinary field, overarching practically all the other domains of application and its integrated approach create the premises of success of development of the field in the next 50 years.

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