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Experience with application of professional software for teaching process design

Václavek Vladimír, Novotná Alexandra, Soběslavová Kamila

Department of Chemical Engineering, Prague Institute of Chemical Technology.
Technická 5, 166 28 Prague 6 - Dejvice, Czech Republic

This paper deals with teaching of process design. Any industrial chemical process can be developed in many variations. In the conceptual process design all possible variations are to be taken into account but all versions which are not feasible or viable have to be excluded as soon as possible. The detailed process design involves all further activities until building up and commissioning the palnt. Despite the fact that the process design is a typical team work, the former case is more or less concerned of chemical engineers, while the latter part is a job for machinery, construction, electrical and control engineers.
In order to be closer to actuall professional activity, the teaching of process design would respond to a following situation encountered in practice. There exists somebody as a licensor, who offers knowledge about the process developed to the stage after the conceptual design. On the other hand there is a contractor who finishes the rest. A scope of this paper is to discuss this new situation when besides commercial simulation programs like PRO/II and ASPEN+ the contractor has at disposal further software tools for improvement of quality and higher productivity of projecting activities. Namely it is a database Comos FEED and a product SmartPLANT.

1. Introduction

The key challenge for chemical engineers in the twenty-first century has been formulated besides the others as it follows [1]:"Design processes and products which are innovative, energy efficient and cost - effective, make the best use of scarce resources and ensure that the waste and adverse environmental impact are minimised". Therefore, teaching of process design seems to be a very important task and there is a question how to do it in the best way.
This paper tends to contribute to discussion about new aspects of teaching and training for process design on various education levels like BS, MS, PhD as well as for courses offered to practice. Authors of this paper have been engaged in this activity during the last two decades. They appreciate possibility to gain some advanced ideas, experience and teaching modules in the framework of TEMPUS project at UMIST, U.K. [2], which have been further arranged and implemented for conditions of the Czech Republic. In order to fulfil the requirements of the Bologna protocol (i.e. two level B.S. and M.S. education system, common for EC) it is necessary to obey conditions of accreditation of degree courses. Plenty of activities are to be carried out e.g. to working out a course syllabus, questionnaires, project guidelines, guidelines to heads of departments,

educational institutions and assessors, etc.

1.1. Conceptual and detailed process design

Naturally the teaching of process design would be as close as possible to solving practical problems. On the other hand some initial background of knowledge has to be obtained first. A generally accepted way how to start up with this discipline is to follow a path of green grass project. A problem formulation in this case specifies some quantity of a particular chemical substance, which could be sold somewhere on the world market for a given price. A process is to be found which is technically feasible and economically viable. The process has to be economic, ecological, safe, energy-saving, controllable, etc.

It is known that nearly any chemical industrial process can be realised up in many variations. In the conceptual process design we would take into account all possible alternatives but exclude all versions without perspective as soon as possible. A result of the conceptual design is one final version if accepted.

Major activities in this stage are namely [3]:

- Choice of reaction path and type of reactor.
- Evaluation of economic potentials in individual steps of the design
- Specification of boundary (external) process streams.
- Development of process topology (a flow- sheet).
- Calculation of material and enthalpy balances.
- Material Safety Data Sheets of components.
- HAZOP (Hazard and Operability study),
- Application of the theory of process integration (pinch technology).
- Sizing (determination of characteristic dimensions of equipment).
- Costing (calculation of equipment and investment costs).

The detailed process design involves all activities after the conceptual design and before erection and commissioning of a plant like:

- Simulation calculation by means of commercial programs.
- Development of PFD and P&ID.
- Lay-out in 2D and 3D.
- Process control strategy. Measurement, sampling and analysis.
- Choice of computation technique for process control.
- Further HAZOP study. Classification of risks, hazard areas. Trip systems.
- Number and qualification of personnel.
- Availability of utilities at battery limits of the process. Other civil facilities.
- Detailed (authorised) economical calculations.
- Modeling of dynamic process behaviour. (Starting up and shutting down).
- Preparation of equipment order sheets e.t.c.

The process design is expressive intellectual activity. Very frequently it can happen that many activities last longer than primarily scheduled. On the other hand management in practice will always tend to accelerate design works as much as possible. The students or candidates would be aware of timetable environment and be prepared to work under stress. The project should have specified successive goals and final targets.

The process design is a typical team activity. Individual team members have different abilities and dispositions and hence they would solve differently difficult partial problems as it is also usual in practice. Each team member should be responsible for accomplishing his/her particular task and cope with communication inside the team and presentation of results. A coordinator (a team leader) has to set up all contributions from individual team members so as to obtain the final required solution.

Creative thinking is emphasized elsewhere as principal presumption of success. More experienced workers can make use of analogy with already solved problems. However this experience is hardly transferable to beginners and it can be gained by participation on solving more design problems. Knowledge of using special mathematical tools is necessary but not sufficient condition how to obtain this experience.

1.2. Other types of problems in the process design

Besides solving the green grass projects one can ecounter other types of problem formulations in practice. They would be also taken into account for further enhancement of teaching e.g.

- Retrofits and revamps of existing plants. Redesign of already existing plants in order to restore originally rejected alternatives which could become viable under new circumstances. This activity needs some experience, in order to make use of unique features of the process under concern.
- Utilisation of process measurements in reference plants for process design. Reconciliation of measured data.
- Energy (water, solvent, hydrogen) saving through process integration (pinch technology). In this case standard flexible procedures have been elaborated. Possibility of setting up the targets (energy, area, economical) is a great advantage.
- Seeking manufacturing programs for some existing facility or even a piece of equipment. This activity needs special wide experience.
- Documentation for authorities concerning various approval procedures and permissions like EIA, IPPC, ISO, Safety report, Feasibility study etc. These materials would be obtained automatically as by-products of the process design provided a special software support is available for this purpose.
- Attention to B. A. T. - the best available techniques. Many alternatives delivered by the conceptual process design at one side contradict with limitations caused by respecting the B.A.T. on the other hand.
- Process design for manufacturing of new chemical specialities, medicaments etc. in low capacity multi-product and multipurpose plants via multi-stage batch operations. A general approach in this case needs some other approach then mentioned above for great capacity plants.
- Implementation of new software packages (e.g. COMOS and SMART), in order to achieve a higher and compatible professional standard of the process design.
- Design and project of great capacity plants with prevailing continuous operations processes which are in principle known and already exist in numerous variations. Both last mentioned aspects are further discussed in more detail.

2. New aspects in the process design

2.1. Process design on the basis licensor-contactor

The following situation concerning the process design has occurred in our conditions which would be also reflected in teaching and training. There are projecting organisations which do not carry out their own process research and development. If they intend and are capable to erect and commission some process plant then they purchase technological know-how from licensors and thus become contractors. The licensors are institutions or companies, very often market leaders, which already realised the particular processes in practice and can offer experience and references. From various reasons they are not interested in doing the particular contract themselves. A typical co-operation between the licensor and the contractor on the level of basic design can be roughly described as follows. Besides description of technology the licensor yields a PDP (Process Design Package), which includes namely information about:

- Process engineering like process design specifications. Process Flow Diagram (PFD), Process and Instrumentation Diagram (P&ID) etc.
- Equipment engineering. List of equipment. Equipment data sheets, Material requisitions, Equipment layouts, Design specifications etc.
- Piping engineering. List of process and utility lines, Piping classes, Piping layouts.

The contractor uses these documents and issues own standard documentation as prescribed in process design and projecting. Typical technological information delivered by the contractor is e.g. availability of utilities on the battery limit and their connection to the process, process measurement and control, process safety, spatial layout in 2-D and 3-D, building up the structures, commissiong the plant etc. Another task is to ensure and provide linkage among individual processes units in a site (in our case of nitrogenous chemistry e.g. complex of ammonia, urea, nitric acid and ammonia nitrate [4]). The contractor does his own policy in marketing and purchasing of equipment, financing the project, providing all necessary approvals from authorities etc. The licensor is responsible for completeness and quality of documentation and the contractor mostly relies on that. However the documentation from licensors need not be perfect and some kind of checking and supervision is necessary. This seems to be an important issue in the process design according to this scheme.

Looking at above given definitions of the conceptual and detailed process design, one can see that the conceptual stage of design, called also as a process study, can be limited or even skipped by the contractor. On the other hand this early stage of the process design is very important for education of chemical and process engineers. In this phase challenging the creative thinking they can realise the fact, that processes can be carried out in numerous variations with possibility of further improvement and perfection. Other professions like machinery engineers, control engineers, building engineers etc. start their jobs when one final version of the process is accepted and approved for realisation. Their activities have more or less routine character with opportunities for algoritmisation and computerisation.

2.2. Professional software products

There are several software tools available and recommended for improvement of quality and higher productivity of projecting activities and seeking opportunities for innovations during the whole life time of processes. Especially two program packages are worth mentioning in this respect and namely Comos FEED offered by Innotec GmbH. [5] and SMART Plant a product of Intergraph Company [6].

As a matter of fact COMOS is an empty database and various kinds of data are to be exported into it. The program package SMART is a final step of the whole activity toward to process design. The SMART requires linkage with COMOS. Fig.1. illustrates the situation. See a new definition of Front-End and Detailed Engineering.

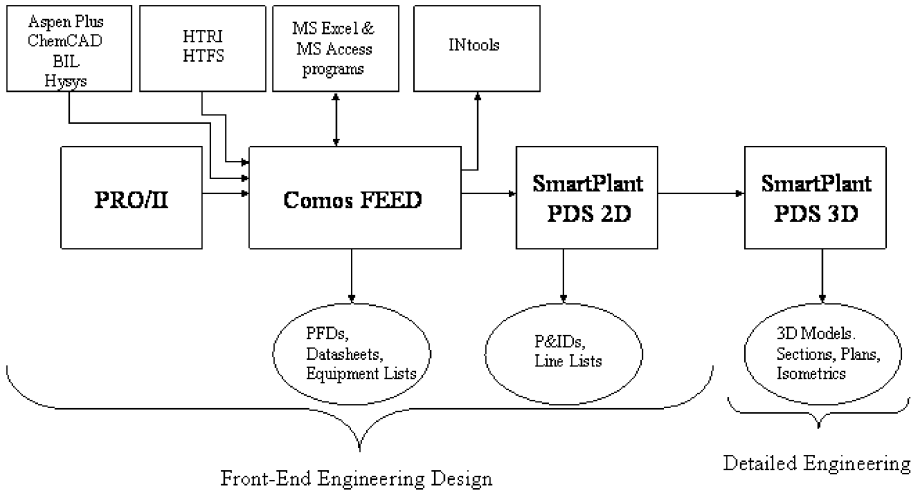

Fig.1. Scheme of design track PRO/II→ComosFEED→SmartPlant.

Comos FEED is an engineering data and document database that provides to integrate Front-End Engineering Design (FEED) activities. Among FEED activities we can comprehend outputs of simulation programs such as PRO/II, Aspen+ [7], Hysys, ChemCAD, then MS Excel and MS Access programs which are entering Comos FEED database. HTFS (Heat Transfer Innovation) are the most integrated Aspentech´s products for physically-based modelling from unit and overall process. Outputs from Comos FEED to SmartPlant are PFDs, Datasheets and Equipment Lists as well as all necessary for SmartPlant.

SmartPlant covers the plant front-end enginnering and detailed schematics design for plant configuration, control systems, and power distribution (to mention just a few). It is beyound the scope of this paper a full description published elsewhere.

2.3. Export of data to ComosFEED

In ideal case the licensor would hand over the documentation to the contractor perhaps in form of filled up database Comos for the required process conditions and any data export could be avoided. This situation is very unlikely in practice and the contractor has to complete Comos database on his own. Logical questions for discussion are

possible utilisation of incompletely filled database and required accuracy of values. Fig.1. also points out to the fact, that besides PRO/II as recommended simulation program for feeding Comos with process data, there are still other commercial and also user´s or pilot programs indispensable as well as databases. The application of material and enthalpy balance calculations from determined [8] and measured [9] data proved to be very effective in this respect.

The first operation of detailed or front-end engineering design is simulation calculation. Its goal is to precise process topology and to provide parameters of process streams. However there is no comment about a source of input data for PRO/II itself. A module for calculation of physical-chemical properties usually involves the most common components in its database and enables to apply advanced methods in physical chemistry. For export of results from preceding stages to Comos the user would be aware of specific terminology and different structures. Information about the process topology cannot be transported but it has to be created in Comos.

3. Acknowledgements

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