Abstract

INTERDISCIPLINARY APPROACH OF CHEMICAL PROCESS ENGINEERING AND ADVANCED CONTROL BASED ON MODELLING, SIMULATION AND ARTIFICIAL INTELLIGENCE TOOLS

My professional development has been engaged in the interdisciplinary fields of Chemical Process Engineering and Systems Engineering which merges Process Control with Process Modelling and Optimization, all using the computer aided tools. Process Control has strong connections with the field of Chemical Engineering and its applications are of major importance for the chemical plant efficient and safe operation for sustainable development.

The research and academic work has been performed on the following main directions:

I. *Modelling in Chemical Process Engineering*

The work aimed to develop models has its roots and motives in the observations I made during the first eight years of working in an industrial chemical plant, when I realised that finding the origin of the inappropriate operation implies the thorough understanding of the process. I became aware of the fact that successul operation of the chemical plant, strongly relying on the control system, is deeply related to the capability of describing its quantitative and qualitative time and space behaviour.

The work I have done in the field of building models and simulators may be grouped in *analytical modelling* and *statistical modelling*. The analytical modelling work can be also divided in modelling systems with *lumped* and *distributed* parameters.

I have developed analytical models for a variety of chemical processes from the field of chemical process engineering, such as:

- Fluid Catalytic Cracking Unit, Waste Water Treatment, Drying Process of Electric Insulators and Batch Distillation, for processes with lumped parameters;
- Pollutant Propagation in Rivers, Forced Convection Drying in Food Slabs, Calcium Carbonate Thermal Decomposition, Drying Process of Electric Insulators and Rotary Calcinator for Soda Ash, for processes with distributed parameters.

The information disclosed by the developed simulators for the distributed parameter systems are valued by the control system design and operation. Revealing the time and space change of the state and output variables of distributed parameter systems relies on models described by partial difference equations. Spatial placement of the measuring devices and actuating elements of the control loops are revealed by these models. At the same time, assessment of the control system performance benefits of the spatial and temporal description. The models have been used for model based control. The research work that was performed in this area has an important potential of further development.

A distinct work was devoted to the statistical modelling based on Artificial Neural Networks (ANNs), due to their prediction and the classification aptitudes for modelling systems in which detailed governing rules are unknown or are difficult to formalise. The prediction aptitude of the ANN relies on its ability of learning, making generalizations and its robust behaviour in the presence of noise. ANNs modelling performance are reinforced by their speed of processing the data. ANNs based models have been used for different processes: Fluid Catalytic Cracking Unit, Waste Water Treatment Plant, Batch Fermentation Bioreactor, Drying Process of Electric Insulators or for simulation of the Electrochemical Impedance Diagrams. Methodologies for the design of the ANN architecture and training procedures have been developed for the considered applications. Feedforward networks with backpropagation training algorithm, radial basis, probabilistic and general regression ANNs have been used.

II. Control in Chemical Process Engineering

The developed models have been used for operation improvement using different control methods. Model Predictive Control is the most promising and appreciated advanced process control methodology used in chemical engineering applications, in standalone or coupled with PID control structures and implemented in either decentralized, supervisory or in multivariable control configurations. Applications have exploited MPC remarkable features consisting in its optimal based way of computing the control law, ability of incorporating constraints in a systematic way, multivariable control approach and prediction capability. MPC of different processes has been investigated based on:

- analytical developed models, such as: MPC of the Fluid Catalytic Cracking Unit, MPC of the Waste Water Treatment Plant, Control of the Soda Ash Calcinator or Control for Counteracting Accidental Pollution in Rivers,
- ANN developed models, such as: MPC of the Fluid Catalytic Cracking Unit, MPC of the Waste Water Treatment Plant, MPC of the Drying Process of Electric Insulators

Fuzzy control for the FCCU, hexamethylene-tetramine reactor and drying process of porous materials have been also studied.

The step response, state space or ANN based models have been used for the prediction of the controlled variable (directly measured or inferred). The way to achieve proper tuning the MPC parameters has been investigated. The adaptive MPC based on scheduled evaluation of the linear model used for prediction of nonlinear processes was explored. Cases of the MPC control in the presence of constraints and using higher number of manipulated than controlled variables were also analysed and applied. Control system design based on feedforward control in either traditional or MPC setup were proposed and successfully used in applications.

III. Data Mining

Another direction of reasearch was the data mining based on ANNs' classification capability (e.g. probabilistic, radial basis, competitive, self organizing maps). It was used for revealing hidden features to be further exploited for chemical process design, control and optimization. Applications have been developed for: Vapour-Liquid Equilibrium Predictions, Antioxidant Activity Prediction and Classification of Teas, Prediction of Thermodynamic Properties, Classification of Wines, Characterisation of Commercial Vinegars, Diagnosing cirrhosis and portal hypertension. Feature selection procedures have been applied and classification results reveal the potential of the developed applications.

IV. Academic work

It was one main aim of my teaching work to use the Systems Engineering approach to the Chemical Process Engineering education where a large area of applications may only be addressed on the basis of the system concepts. The Computer Aided Chemical Process Engineering program, at bachelor and master level, developed at the Faculty of Chemistry and Chemical Engineering, has been sustained by teaching courses such as: Systems Theory, Basic Process Control, Advanced Process Control, Mathematical Modelling and Artificial Intelligence with applications in the field of chemical engineering.

Advanced Chemical Process Engineering Master Program was coordinated and developed to gain international participation (e.g. students from India, Turkey, Vietnam, Egypt, Kazakhstan, Irak, Algeria).

I supervised 48 bachelor theses and 32 master theses of the students who graduated the chemical engineering programs at the Faculty of Chemistry and Chemical Engineering. I have also supervised the education and research activities for 11 foreign students having internships in the Chemical Engineering field. Two post-doctoral Chemical Engineering students have worked under my supervision and I was member of the advisory committees for 10 PhD students. As referent I participated to the evaluation committees of 14 PhD theses having topics in the chemical engineering (13) and systems engineering (1) fields, from: University Politehnica of Bucharest, Politehnica University of Timişoara, Petroleum-Gas University of Ploieşti, Technical University of Cluj-Napoca and Babeş-Bolyai University of Cluj-Napoca.

My future research work will be placed at the overlapping area of the Chemical and Systems Engineering fields, as modelling and optimization have become parts of the control system design and control turns to play major importance in the chemical process design and operation. The complex chemical process engineering systems featuring nonlinearity, multivariable character and uncertainty, associated to equipment and operation constraints make the control a difficult but exciting task. A team of motivated and inspired PhD students would offer the essential ingredient to approach the research work in order to comply with these multiple challenges.
The main directions of the future research work with potential PhD students are:

- *Control of Processes with Distributed Parameters for Chemical Plants Applications* (modelling using CFD tools; designing and tuning the controllers for stability, in the presence of uncertainty; optimal allocation of the sensors, decentralized control; model reduction; development of model based estimators),
- *Advanced Model Based Control and Optimization with Applications in Chemical and Environmental Engineering fields* (internal model control, MPC, MPC tuning, MPC with multiple models, MPC using ANN models and fuzzy logic, Nonlinear MPC, reducing computation load of MPC, economic MPC, MPC with genetic algorithms, swarm algorithms, ant colony optimization, Pareto optimality),
- *Application of Computational Intelligence (CI) and Data Mining Tools in Chemical Process Operation and Control* (hybrid modelling First principle-ANNs-Fuzzy logic, optimization using genetic algorithms, swarm algorithms, classifications based on ANNs and Fuzzy logic, nonlinear model based control).

The future education work will involve the development on three layers:

- The *basic layer* will be devoted to the work with students from the bachelor and master programs (basis of the pyramid in the higher education hierarchy),
- The *intermediate layer* for the development of the research group (CAPE Research Centre) that merges the knowledge and experience of older and young members in the field of the chemical process modelling, control and optimization,
- The *higher layer* it is situated the level of development of the group of PhD students (as potential PhD coordinator) and the affiliation to the Chemical Engineering PhD school (selection of human resources, development of the infrastructure, participation to project competitions for obtaining financial support, collaboration with national and international education and research groups, increasing visibility of the Chemical Engineering PhD school by applications solving real life problems in industry or society and by producing relevant publications).