Chemical Process Modeling and Control Research Center

iacocca Hall, 111 Research Drive; 610-758-6654

Mayuresh V. Kothare, Ph.D., codirector; William L. Luyben, Ph.D., codirector; Hugo S. Caram, Ph.D.; William E. Schiesser, Ph.D.; Eugenio Schuster Ph.D.; James T. Hsu, Ph.D.

The mission of the Chemical Process Modeling and Control Research Center at Lehigh University is to advance the theory and application of feedback control techniques, dynamic modeling, optimization and automation, and to apply these tools to a range of chemical and biological systems. A key execution strategy involves close collaboration with industrial partners to identify and solve technological relevant automation problems.

The Center was established in January 1985 through the efforts of faculty members of the chemical engineering department at Lehigh University, leading industrial processing companies, the Ben Franklin Partnership Program of the Commonwealth of Pennsylvania, coupled with the organizational and financial support of the National Science Foundation (NSF).

The center provides a unique atmosphere for fundamental research, development of specific techniques, application to real industrial processes, and opportunities for advanced education (M.S. and Ph.D.) in chemical process modeling and control for academics and industrial practitioners. Facilities are available for real time testing of new algorithms in experimental process units, development of dynamic simulations of real processes, and the close collaboration with researchers in several other fields of chemical processing.

Interdisciplinary collaboration is encouraged with other research groups, centers, or institutes engaged in biotechnology, polymer processing, environmental science, applied statistics, signal processing, chemical reaction engineering, and process design.

EDUCATION
An integral part of the center is the commitment to conduct an outstanding program dedicated to the education of undergraduate and graduate students. The center has and continues to attract top quality students from a large group of well recognized international universities. In addition, each year several industrial companies send employees to receive advanced training and engage in research efforts for particular company technical requirements.

FACULTY
The center brings together several faculty members from different engineering disciplines in the university engaged in the research and educational efforts of the center. Visiting faculty from other well recognized universities supplement these researchers and provide opportunities for diversity of thinking and innovative research. All of the associated faculty members are recognized around the world as leaders in their respective fields of specialization. They also serve as consultants to a variety of industries.

FACILITIES
The Center is located in Iacocca Hall on the Mountaintop Campus of Lehigh University. This building represents a unique facility available to the center as well as the chemical engineering department and the Emulsion Polymers and Bioprocessing Institutes. The center has the use of several dedicated computer facilities with numerous workstation computers continuously available to the students, faculty, and staff. In addition to the local computing network, the center's researchers have access to the Lehigh University central computing facilities and its outside links to other worldwide computing systems and data networks. The center has several laboratories with sophisticated equipment dedicated to process control research work.

AREAS OF RESEARCH
The research activities of the Center span a wide spectrum of problems in large complex chemical process design, dynamical analysis and control, as well micro and nanoscale complex process development, evaluation, dynamical analysis and control. A recently added area of research studies the role of feedback control in biological systems with particular emphasis on neuronal systems encountered in neuroscience and neurology. The research themes emphasize a combination of new theoretical developments, new applications and translation of new theoretical developments to practical problems.

1. Synthesis and PlantWide Control
   During the last decade Center faculty have done pioneering work in the area of plantwide control, which has resulted in the only textbook that covers this important area. There continue to be a number of projects in this area.
   a. On Demand Control of Processes with Multiple Products: This project studies the design and control of processes in which consecutive reversible reactions produce multiple products. The demand for these products can vary, so the process and its control system must be able to produce exactly the desired amount of each individual product. An ideal system has been studied first in which the effect of equilibrium constants and volatilities can be explored. A real chemical system is also being studied (the production of methyl amines).
   b. Design and Control of Tubular Reactors Systems: Adiabatic gasphase exothermic reactions are often carried out in tubular reactors. There are several types of systems: a single adiabatic reactor, multiple adiabatic reactors in series with either intermediate cooling or "cold shot" cooling (mixing some cold feed with the hot reactor effluent) and a cooled tubular reactor. These alternatives are being studied in terms of both steadystate design (which has the lowest total annual cost) and dynamic controllability (which provides the tightest temperature control in the face of disturbances).

2. Dynamics and Control of Distillation
   Reactive distillation is an emerging area in chemical engineering because it offers potential savings in capital and energy costs in some systems, particularly for reversible reactions. A recent project explored several reactive distillation systems: ETBE, methyl acetate, TAME, ethylene glycol and metathesis of pentene. The steadystate economic designs of these systems were studied. Then their dynamics and control were explored. Different types of chemical systems require types of control structures. These columns are sometimes operated using of an excess of one of the reactants and sometimes using exact stoichiometric amounts of the two fresh reactant feeds. Both the process design and the control scheme are different with these two scenarios.

3. Convex Optimization Techniques in Linear and Nonlinear Process Control
   The last few years have seen the emergence of a new class of optimization problems that have been variously referred to as Linear Matrix Inequalities (LMIs), semidefinite programming (SDP) problems and convex problems. We were one of the first groups to explicitly show the applicability of LMIs in process control by reformulating the modelbased predictive control (MPC) algorithms as LMI problems. There are several classes of problems involving control of systems subject to constraints that are amenable to LMI formulation. These include efficient offline MPC for fast sampling time processes, observerbased nonlinear, MPC, multimodel transition control using MPC, antiwindup, moving horizon estimation and evaluation of robustness, i.e., the impact of model uncertainty on controller performance. These new control algorithms are being tested on numerous application platforms.

4. Multi-Model and Hybrid Systems Analysis and Control
   Hybrid and multimodel systems are a class of systems in which there is interaction between continuous dynamical behavior of systems with discrete switching behavior. For example, systems described by piecewise linear multiple models are continuous and linear within a prescribed region and switch to a different linear model description in a different prescribed region of the statespace. Other examples include switches and overrides that switch one of a family of controllers into the closedloop, based on the operating space and control objective. Our research in this area has focused on two broad problems (1) control of systems described by multiple piecewise linear models; (2) formulation of saturated systems as switched/piecewise linear models and subsequent antiwindup controller design using piecewise quadratic functions. We demonstrated, through a case
study, the control of a highly nonlinear solution copolymerization reactor using multimodel switching MPC. We have also shown how an appropriate antiwindup controller synthesis problem can be formulated using piecewise quadratic Lyapunov functions.

5. Dynamics and Control of Micro and Nanochemical Systems
Microchemical systems are a new generation of miniature chemical systems that carry out chemical reactions and separations in precisely fabricated three-dimensional microreactor configurations in the size range of a few microns to a few hundred microns. Typical microchemical systems combine fluid handling and reaction capabilities with electronic sensing and actuation, are fabricated using integrated circuit (IC) manufacturing techniques and use silicon and related IC industry materials, polymers, ceramics, glass or quartz as their material of construction.

The goal of this integrated research and education program is to study the unique dynamical properties of such integrated microchemical systems and to develop a framework for designing implementable feedback control techniques for this class of microsystems. Concepts for distributed and boundary control theory will be employed to study the model-based feedback control formulation of microchemical systems and to develop a technical framework for microsystem controller design. The Integrated Microchemical Systems Laboratory (under the direction of Professor M.V. Kothare) conducts this research as part of the Center.

6. Control of Biomedical Systems: We are currently working on applying control techniques to emerging problems in biomedical engineering, in particular, in neuroengineering. This involves developing models of ensembles of neurons in the human brain and use of such models in optimizing closed loop neuroprosthetic rehabilitation strategies.

For more information, contact Mayuresh V. Kothare (coDirector) or William L. Luyben (coDirector), Center for Chemical Process Modeling and Control, Iacocca Hall, Lehigh University, 111 Research Drive, Bethlehem, PA 18015-4791, (610) 758-6654, fax (610) 758-5297, email: mayuresh.kothare@lehigh.edu, wll0@lehigh.edu.