Control of Nonlinear Distributed Process Systems: Recent Developments and Challenges

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Introduction

While most undergraduate process control courses still deal with dynamics and control of lumped chemical processes using linear transfer function models, key technological needs in growth areas such as semiconductor manufacturing, nanotechnology, biotechnology, and unmanned aerial vehicles have motivated extensive research on analysis and control of complex nonlinear distributed systems across all engineering disciplines. From a control point of view, the distinguishing feature of complex distributed systems is that they give rise to nonlinear control problems that involve the regulation of highly distributed control variables by using spatially-distributed control actuators and measurement sensors. Thus, complex distributed systems cannot be effectively controlled with control methods which assume that the state, manipulated and to-be-controlled variables exhibit lumped behavior or with linear control algorithms derived on the basis of linear/linearized distributed models.

Table 1: Distributed Control Problems and Applications

Distributed Control Problems	Applications
Control of spatial profiles	*CVD, Etching, Crystal growth, Packed-bed reactors*
Conrol of size distributions	*Aerosol production, Crystallization, Emulsion polymerization, Cell cultures*
Control of fluid flows	*Fluid mixing, Wave suppression, Drag reduction, Separation delay*
Control of material microstructure	*Thin film growth, Nano-structured coatings processing*

There exists a wide range of distributed control problems (Table 1); in what follows, we focus on two representative classes of industrially-important distributed control problems to provide some insight into the origin and nature of such problems and motivate the need for nonlinear feedback control based on fundamental distributed models.

Control of Spatially-Distributed Profiles. A typical example of this class of problems is the control of the temperature profile across the wafer in the single-wafer rapid thermal chemical vapor deposition (RTCVD) process to reduce film deposition spatial nonuniformity. RTCVD uses several sets of lamps to radiatively heat the wafer from room temperature to about 1,200 K at very high heating rates, and then keep it at the high temperature for a short time to run the deposition reactions. While this sharp increase in the wafer temperature reduces significantly the overall processing time (usually less than a minute) and the diffusion length, thereby preserving dopant concentration profiles from previous steps, it may lead, especially for large wafer dimensions, to significant nonuniformity of the wafer temperature profile. This, in turn, may lead to film deposition uniformity that does not meet the tight requirements set by the industry (SIA, 1997). This technological need and the complex character (nonlinearities, spatial variations, batch nature) of the RTCVD process motivate the need to control the wafer temperature profile using a nonlinear feedback controller based on a distributed process model.

Control of Particle-Size Distributions. A typical example of this class of problems is the control of titania aerosol reactors to achieve a nearly monodisperse particle-size distribution (Kalani and Christofides, 2000); this is required for titania pigments to obtain the maximum hiding powder per unit mass. Titania aerosol production is a very complex and highly nonlinear process that involves particle formation from gases through chemical reaction and nucleation, particle growth through condensation, coagulation and coalescence, and particle transport. Over the last 20 years, there have been major advances in understanding these phenomena and in quantifying their effect on the shape of the aerosol size distribution using population balances. These fundamental advances, together with recent developments in real-time measurement of aerosol size distributions using laser scattering techniques, make nonlinear model-based feedback control of aerosol size distribution feasible and practical.

Fundamental modeling of distributed process systems typically leads to nonlinear distributed parameter systems (DPS) ranging from hyperbolic and parabolic partial differential equations (PDEs) for transport-reaction processes, to Navier-Stokes equations for fluid flows, and to integro-differential equations for particulate processes. While such systems can accurately predict nonlinear and distributed dynamic behavior, their infinite-dimensional nature does not allow their direct use for the design of nonlinear controllers that can be readily implemented in real-time with reasonable computing power. Conventional approaches to discretization of nonlinear DPS involve the use of finite-difference/finite-element techniques and lead to approximate systems of thousands of ordinary differential equations which are inappropriate for controller synthesis and real-time controller implementation. This limitation has been the bottleneck for model-based synthesis and real-time implementation of nonlinear feedback controllers to distributed processes.

Recent Developments

Over the past two decades, research on dynamics of nonlinear DPS has led to the discovery that the dominant dynamic behavior of many distributed process systems can be characterized by a small number of degrees of freedom. Examples of this fundamental property include the discovery of coherent structures in turbulence (Lumley, 1981), the formation of patterns in various diffusion-reaction processes (Shvartsman and Kevrekidis, 1998), the decomposition of chaotic mixing flows using symmetry concepts (Franjione and Ottino, 1992), and the occurrence of oscillatory behavior in continuous crystallizers (Jerauld et al., 1983). The discovery of dominant (low-dimensional) dynamic behavior has led to the introduction of rigorous mathematical concepts (e.g., inertial manifold (Temam, 1988)) to capture this type of behavior and the development of advanced model reduction techniques for deriving low-dimensional approximations that accurately reproduce the dynamics and solutions of various classes of nonlinear infinite-dimensional systems. Such techniques include Galerkin's method with data-based construction of the basis functions (empirical eigenfunctions) and nonlinear Galerkin methods (Shvartsman and Kevrekidis, 1998). On the other hand, control theory for lumped nonlinear processes has advanced to a stage where powerful controller synthesis algorithms are available for broad classes of nonlinear systems based on differential geometric (Kravaris and Arkun, 1991) and Lyapunov (El-Farra and Christofides, 2001) techniques.

Over the past five years, major breakthroughs in control of nonlinear DPS have been accomplished by bringing together concepts from nonlinear dynamics of infinite-dimensional systems and nonlinear control theory. Specifically, research has led to the development of a general and practical framework for the synthesis of nonlinear low-order feedback controllers for broad classes of nonlinear infinite-dimensional systems that arise in the modeling of transport-reaction processes (parabolic PDEs with fixed and time-dependent spatial domains) (Christofides, 2001), fluid flows (Navier-Stokes equations) (Baker et al., 2000) and particulate processes (population balances) (Chiu and Christofides, 1999). Within the developed framework, the infinite-dimensional closed-loop system stability, performance and robustness properties have been precisely characterized in terms of the accuracy of the approximation of the low-dimensional models. Owing to the low dimensional structure of the controllers, the computation of the control action involves the solution of a small set of ordinary differential equations (ODEs), and, thus, the developed controllers can be readily implemented in real time with reasonable computing power.

To explain the main features of the new approach, we now focus our discussion on nonlinear control of parabolic PDE systems (see Christofides (2001) for a detailed treatment). Such systems involve spatial differential operators whose eigenspectrum can be partitioned into a finite dimensional "slow" set (which includes eigenvalues that are close to the imaginary axis) and an infinite dimensional "fast" complement (which includes eigenvalues that are far in the left half of the complex plane). This separation of the eigenvalues implies the existence of low-dimensional structures (inertial manifolds) that capture the dominant dynamics of the PDE system, and suggests addressing the controller synthesis problem on the basis of low dimensional ODE approximations of the PDE system. Motivated by this, the standard approach to control of parabolic PDEs involves the application of Galerkin's method to the PDE system to derive ODE systems that describe the dynamics of the dominant (slow) modes of the PDE system, which are subsequently used as the basis for the synthesis of finite-dimensional controllers. The main disadvantage of this approach, especially in the context of nonlinear parabolic PDEs, is that the number of modes that should be retained to derive an ODE system that yields the desired degree of approximation may be very large leading to complex controller design and high dimensionality of the resulting controllers.

To overcome the problem of high dimensionality, a singular perturbation formulation of Galerkin's method, which takes advantage of the separation of the eigenspectrum of the spatial differential operator and leads to a natural formulation of the concept of inertial manifold, has been proposed (Christofides, 2001). While the explicit construction of an inertial manifold is an almost impossible task for any practical application, the developed singular perturbation formulation provides an easy-to-use procedure for the construction of approximations of the inertial manifold (called approximate inertial manifolds (AIMs)) of the PDE system. The AIMs are utilized for the derivation of accurate low-dimensional approximations of the PDE system. These low-dimensional approximations are then used for the synthesis of nonlinear feedback controllers, employing geometric control methods that enforce the desired stability, performance, and robustness properties in the infinite-dimensional closed-loop system. Using singular perturbation theory, the transient performance of the closed-loop system is precisely characterized in terms of the degree of separation between the slow and fast eigenvalues of the spatial differential operator. Within the developed framework, nonlinear controller designs have been proposed that deal directly with the key practical issues of uncertainty in model parameters, constraints in the capacity of control actuators, and control actuator/measurement sensor dead time. Furthermore, to enlarge the class of transport-reaction processes for which the proposed methods are applicable, extensions of the nonlinear model reduction and control methods to parabolic PDE systems with nonlinear spatial differential operators and boundary conditions, as well to systems with time-dependent spatial domains, have been addressed (Christofides, 2001).

In addition to the above approach, other approaches for control of nonlinear PDE systems have been pursued, including distributed control using generalized invariants (Palazoglu and Karakas, 2000) and concepts from passivity and thermodynamics (Ydstie and Alonso, 1997), and they have led to systematic controller design methods.

The theoretical development of the nonlinear control methods has been accompanied by practical applications to several distributed process systems using high-fidelity simulated models to solve several industrially important distributed control problems. These applications include control of the wafer temperature profile in the RTCVD process and crystal thermal gradient profile in the Czochralski crystal growth process (Christofides, 2001), control of size distribution in a continuous crystallizer (Chiu and Christofides, 1999) and a titania aerosol reactor (Kalani and Christofides, 2000), as well as suppression of wavy behavior (Armaou and Christofides, 2000). Extensive comparisons of the nonlinear control algorithms with linear control schemes have demonstrated the effectiveness and superiority of nonlinear control, motivating further research on both theoretical problems and application studies in this rapidly expanding field.

Research Challenges

The objective of this section is to provide a presentation of the main theoretical and practical challenges on analysis, design, and control of nonlinear distributed process systems.

Integration of Design and Control. It is well-known that simple modifications in design may lead to processes that are easier to control (Stephanopoulos, 1983). This realization has motivated extensive research on the integration of process design and control for lumped chemical process systems. This research has led to the introduction of basic concepts (controllability and flexibility) to account for control considerations at the design stage and the development of systematic methods for integrated process design and control within an optimization framework. Through numerous applications, the integrated approach to design and control has been shown to be superior to the traditional sequential approach (i.e., first design, then control). In the context of distributed process systems, however, the integration of design and control has received very little attention. One of the main obstacles for addressing this problem is the lack of computationally efficient algorithms for solving infinite dimensional optimization problems arising in the context of integrated optimal design and control problems for distributed process systems.

In this area, future research should target the development of a rigorous and practical framework which will systematically and simultaneously address the design of the process (e.g., shape and size of a reactor), the synthesis of the control configuration (choice of controlled, measured, and manipulated variables) and controller (control algorithm and parameters), and the controller implementation (measurement sensor and control actuator type and location). Such an approach will identify the true limitations on the best achievable process performance, and will produce processes and control systems whose dynamics "cooperate" to achieve the desired performance specifications with minimal energy use. To this end, research should focus on the introduction of appropriate controllability and flexibility concepts for distributed process systems, the development of an appropriate mathematical framework for analyzing infinite-dimensional optimization problems, the construction of computationally efficient algorithms for their solution using nonlinear model reduction techniques, and the computation of optimal locations for control actuators and measurement sensors.

Analysis and Control of Hybrid Distributed Process Systems. An important area of future research will be the control of distributed process systems whose transient behavior combines both continuous and discrete features. While continuous behavior arises from the underlying physico-chemical phenomena, discrete phenomena typically arise from discontinuities of the basically continuous dynamics (e.g., phase changes, flow reversal), instrumentation with discrete actuators and sensors (e.g., on/off valves, motors with constant speed, binary sensors), or from logical rules for supervisory and safety control (e.g., switching between various control modes). Currently, the abundance of hybrid phenomena in many chemical processes together with the need to design control and supervisory schemes for such processes has motivated significant research on the analysis and control of hybrid lumped systems such as switched systems and mixed logical dynamical systems (Bemporad and Morari, 1999). For their distributed counterparts, however, virtually no research has been done, mainly due to the limited progress in the area of hybrid lumped systems. One of the main obstacles here is the variable structure or changing dynamical nature of hybrid systems making them more difficult to analyze or control.

Future progress in the analysis and control of hybrid lumped systems together with the recent developments on order reduction and control of continuous-time distributed systems will make the analysis and control of hybrid distributed systems an important area of future research. In this area, future research should focus on extending the available concepts and tools used to analyze the stability, controllability, and observability properties of purely continuous-time distributed systems to treat combined discrete-continuous systems. Furthermore, research should focus on the development of a systematic approach for the control of hierarchical distributed hybrid systems, including the integrated synthesis of "lower level" continuous controllers and "upper level" switching laws that orchestrate the transition between different control actuators, measurement sensors, and control algorithms.

Control of Material Miocrostructure Using Multiscale Distributed Systems. In addition to achieving spatially uniform deposition of thin films in chemical vapor deposition processes, one would like to control film properties such as microstructure and composition that characterize film quality. While deposition uniformity control can be accomplished on the basis of continuum type distributed models, precise control of film properties requires multiscale distributed systems that predict how the film state (microscopic scale) is affected by changes in controllable process parameters (macroscopic scale). Multiscale distributed systems constitute coupled molecular models, such as Monte Carlo and molecular dynamics simulations, that capture the evolution of microstructure formation and growth (including nucleation, cluster-cluster coalescence, adsorbate-adsorbate interactions, and impurities) and continuum type distributed models, based on conservation equations of continuity, momentum, energy and species, that describe spatiotemporal process behavior in macroscopic time and length scales. While multiscale modeling provides a computationally attractive alternative with respect to direct modeling of the entire deposition process using a molecular model, it still leads to dynamic models that cannot be solved fast enough for real-time estimation and control purposes. Therefore, future research within this area should focus on the study of the dynamics of multiscale distributed models, the development of order reduction techniques for constructing low-order models that describe film properties directly from microscopic (Monte Carlo and molecular dynamics) film simulations (see Raimondeau and Vlachos (2000) for recent results on this problem), and the integration of multiscale models, advanced sensing capabilities for online thin film microstructure/composition monitoring, and control theory to develop control systems that can be implemented in real time.

Control of Nanoparticle Synthesis and Processing. While some recent efforts have been done on control of size distribution in aerosol reactors, the problem of developing an integrated approach to real-time monitoring and control of nanoparticle synthesis in aerosol processes remains largely unresolved. In addition to shaping size distribution, feedback control may be used to achieve the desired particle morphology, composition, and degree of agglomeration that influence subsequent processing and product properties. Furthermore, real-time control of nanoparticle processing systems, e.g., thermal spray processing of nanostructured coatings using nanosized powders, has not been attempted. The inherently nonlinear and distributed nature of the processes involved in nanoparticle synthesis and processing provides excellent opportunities for the implementation of real-time nonlinear feedback control based on distributed models. Recent advances in online particle-size distribution measurement including laser absorption scattering and probe sampling techniques provide the means for achieving this goal. Similar to the problem of controlling thin film microstructure, a multiscale approach is needed to address the control of nanoparticle synthesis and processing. Thus, major challenges include the development of low-order approximations of multiscale models linking macroscopic scale (e.g., thermal spray process) and microscopic scale (e.g., evolution of coating microstructure), and the integration of models, measurements, and control theory for particulate processes to develop real-time measurement/model-based feedback control. The future emphasis of U.S. research on nanotechnology is expected to provide a strong driving force for studying feedback control of nanoparticle synthesis and processing (Siegel et al., 1999, Chapter 3).

Analysis and Control of Bio-Systems. Recent advances in numerical methods, coupled with the development of user-friendly software tools (such as FEMLAB) for the numerical simulation of distributed systems could have a significant impact on analysis of complex biological systems. In this direction, an example is the recent work of our group (El-Farra et al., 2000) on the computational modeling of the consumption of Nitric Oxide (NO), a molecule responsible for regulating blood pressure in humans and animals, in the micro-circulation. In this work, detailed distributed modeling of the diffusion and reaction of NO in the blood, together with available experimental data, has allowed us to identify and quantify the various sources of resistance to NO transport in the blood. These findings could have significant clinical implications for treatment of several diseases attributed to imbalances in NO transport. In addition to analysis of bio-systems, there are, at least, two more challenging problems in biotechnology where recent results on control of nonlinear DPS could have an impact. First, order reduction techniques for distributed systems, especially methods for the computation of empirical eigenfunctions (dominant spatial patterns) from a large set of solutions, could play an important role in the development of systematic data compression algorithms for the vast amount of data coming out of the various genome projects. Second, the recent results on nonlinear order reduction and control of population balance models, together with recent advances in online flow cytometry of cell populations, could lead to the development of nonlinear feedback control systems for real-time control of cell distributions (see Daoutidis and Henson (2001) for a review of results in this area).

Control of Fluids: Drag Reduction, Separation Control and Mixing Enhancement. Recent advances in manufacturing of control actuators (e.g., blowing/suction, synthetic jets) and measurement sensors (e.g., shear stress sensors) make reactive flow control of aerodynamic flows for frictional drag reduction and delay of separation a very real possibility. Within an open-loop control setting, recent studies have shown that small devices with relatively little energy input can be extremely effective in influencing a flow field, motivating significant research efforts on closed-loop feedback control of fluids (see Jacobs (2000) for several reports of recent results in this area). The ultimate goal of this research would be to replace the traditional hinged aircraft control surfaces, such as flaps and ailerons, with active flow control devices. To reach this goal, future research should focus on the development of systematic control strategies that exploit the natural behavior of a flow field, to delay separation and reduce drag. Advances in control of hybrid distributed systems could play an important role in developing algorithms for switching, based on flight conditions, between different control actuators and measurement sensors placed at different spatial locations to achieve the desired control objectives.

In addition to drag reduction and separation control, the theory for control of fluids may be used to enhance the quality of mixing of two or more fluids. Good mixing is essential in many applications, for example, mixing of air and fuel in combustion engines to improve process performance. While dynamical systems theory and symmetry concepts have been used to analyze mixing, the problem of using external forcing to generate a flow that mixes well has not been studied. In this direction, research should focus on the quantification of mixing, the formulation of appropriate control objectives, and the design of feedback controls that exploit the natural tendency of flows to mix to achieve the desired degree of mixing with minimal energy use. Recent developments on feedback control of Navier-Stokes equations could play a key role in addressing this important problem.

Concluding Remarks

Control of nonlinear distributed process systems is a cross-disciplinary and rapidly growing research area that brings together fundamental modeling, numerical simulation, nonlinear dynamics and control theory. While recent advances have led to systematic methods for the design of easy-to-implement nonlinear feedback controllers for broad classes of nonlinear DPS, the increasing need to achieve feedback control of material microstructure, nanoparticle synthesis, cell distributions, and fluid flows provides a large number of new and intellectually-challenging problems. Solutions to these problems could have a significant impact in important application areas such as semiconductor manufacturing, nanotechnology, biotechnology, reaction engineering, fluid mixing, and aerospace vehicles. In addition to technological needs, several other factors bode well with the increasing interest in and practical impact of control of nonlinear distributed process systems including: (a) the development of easy-to-use software such as FEMLAB that makes distributed system modeling, order reduction, and control routine and easy-to-incorporate in the chemical engineering curriculum, as well as in an industrial environment; (b) the availability of low-cost computing power that allows efficient and fast simulation of complex distributed systems; (c) recent developments in sensors and actuators that make distributed control of spatial profiles, size distributions, microstructure, and fluids feasible and practical; and (d) the current funding trends towards analysis and control of complex processes. The integration of distributed system modeling, simulation, and control into the chemical engineering curriculum will be essential for chemical engineers to play an important role in this rapidly expanding field.

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