Chemical Engineering Seminars – HT 2007

Week 7: Tuesday 27 February, 4:15-5.15 pm
Lecture Room 2, Thom Building, Engineering Science

Optimization and Control of Multiscale Process Systems

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Abstract

With advances in advanced materials processing and demand for high performance devices, allowable manufacturing tolerances are getting increasingly stringent, and process design and control methodologies with ability to control product microstructure are required.

Advances in computing capabilities and optimization algorithms have, in principle, made it possible to design complex processes that are optimal with respect to certain economic criteria. An underlying requirement is that a computationally tractable mathematical model capable of describing the dynamic evolution of the process up to microscopic detail is available. However, a wide variety of processes relevant to materials industry involve phenomena whose characteristic length and time scales are separated by several orders of magnitude, necessitating different descriptions at different length and time scales. Traditionally these processes are modeled through continuum laws, and microscopic phenomena are incorporated through the ``mean-field" approach, which neglects all of the microscopic information that is indispensable if control/optimization at microscopic level is desired. Atomistic simulations (which naturally describe phenomena at all relevant length-scales), on the other hand, are computationally too expensive to be applied at spatial and temporal scales over which physical processes operate.

Motivated by the above, we address the issues arising during optimization and control of multiscale distributed processes where the cost functional depends on both macroscopic and microscopic behavior of the process. By confining the computationally demanding atomistic simulations only to domains where microscopic resolution is required and employing continuum models for the rest of the physical domain the computational requirements of the model may be reduced significantly. The presence of constraints in the form of Partial Differential Equations (PDEs) and stochastic descriptions of the microscopic properties that are unavailable in closed form, however, not only prohibit the use of standard search algorithms for optimization but also render the problem computationally expensive.

We have developed methodologies, based on proper orthogonal decomposition and in-situ adaptive tabulation, that allow formulating optimization problems which are capable of addressing optimization objectives ranging from microscopic to macroscopic scales and simultaneously keeping the problem computationally tractable.

Towards nonlinear controller synthesis, we combine these microscopic simulations with an off-line identification scheme to circumvent the issue of model unavailability and design controllers that are capable of controlling the expected behavior of the process. The applicability of these methodologies is demonstrated for (a) quality control of thin film deposition through the Metal

Organic Vapor Phase Epitaxy (MOVPE) process with a two-fold process objective; minimization of the spatial variations of the thickness of the deposited film across the substrate (macroscopic objective) while accounting for the effects on the roughness (our microscopic objective), and (b) towards the optimization and control of the catalytic oxidation of CO on Pt surfaces..

Bio-sketch

Antonios Armaou was born in Athens, Greece, in 1972. He received the Diploma in Chemical Engineering degree from the National Technical University of Athens, Greece, in 1996, and the Ph.D. degree in Chemical Engineering from the University of California, Los Angeles, in 2001. From 2001 to 2002, he held a postdoctoral research position at Princeton University, after which he joined the faculty of the Chemical Engineering Department at Pennsylvania State University where he currently is Assistant Professor.

His theoretical research interests include nonlinear and robust control, and model reduction, design and control of nonlinear distributed parameter and multiscale process systems, with applications to chemical processes, advanced materials and semiconductor processing, fluid flows and biological and biomedical systems. He has coauthored more than twenty five journal publications and thirty conference proceedings papers. Dr. Armaou's research work has received several awards including the O. Hugo Schuck Best Paper Award (with P. D. Christofides) given by the American Automatic Control Council in 2000. He is the recipient of a Research Initiation Award from the ACS-Petroleum Research Fund in 2006 and a CAREER award from the National Science Foundation in 2006. He is currently an associate editor of the IEEE Control Systems Society conference editorial board.