

Faculty of Engineering and Applied Science Chemical Engineering Seminar Series



Uncertainty analysis tools applied in multiscale process systems and integration of design and control

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ABSTRACT

The aim of this talk is to present recent tools developed in my research group for multi-scale process systems under uncertainty and simultaneous design and control.

Microelectronic market imposes tight requirements upon thin film properties, including specific growth rate, surface roughness and thickness of the film. In the thin film deposition process, the microscopic events determine the configuration of the thin film surface while manipulating variables at the macroscopic level, such as bulk precursor mole fraction and substrate temperature, are essential to product quality. Despite the extensive body of research on control and optimization in this process, there is still a significant discrepancy between the expected performance and the actual yield that can be accomplished employing existing methodologies. This gap is mainly related to the complexities associated with the multiscale nature of the thin film deposition process, lack of practical online *in-situ* sensors at the fine-scale level, and uncertainties in the mechanisms and parameters of the system. In this talk, I will present the recent efforts performed in my group to improve the operability and performance of this process using robust optimization and control strategies that can explicitly account for uncertainty in the multiscale model parameters. Power series expansion (PSE) has been used in this research to quantify the variability in the outputs due to parameter uncertainty. Also, closed-form models describing the dynamics between the key input and output variables for this process has been identified and used for on-line control applications. Outcomes from this research have shown that it is possible to develop efficient strategies that enable accurate online control of the key properties of a multiscale system in the presence of model-plant mismatch.

Simultaneous design and control is an attractive alternative to perform the optimal design of chemical processes while considering the process dynamics in the analysis. Implementation of this strategy will result in the specification of optimal (economically attractive) plant designs that are dynamically feasible in the presence of critical realizations in the disturbances and uncertain model parameters. This talk will present the recent methodologies developed in my group in

this field. One of the methods is based on the concept of the back-off approach, where the key idea is to move away (back-off) from the optimal steady state design, which is often found to be dynamically inoperable due to the process disturbances, process dynamics and model parameter uncertainty. The key challenge is to determine the magnitude of the back-off needed to accommodate the transient operation in presence of disturbances and parameter uncertainty. This approach focuses on calculating various optimal design and control parameters by solving various sets of optimization problems using mathematical expressions obtained from PSE. These approximations are used to determine the direction in the search of optimal design parameters and operating conditions required for an economically attractive dynamic feasible process. A methodology that performs the integration of design, scheduling and control to optimally design multiproduct chemical processes under uncertainty will also be presented in this talk. The decisions involved in this analysis encompass design parameters, e.g., optimal and equipment sizes, control parameters, e.g., optimal controller tuning parameters, and scheduling decisions, which include the identification of optimal transition trajectories and the optimal sequence of production for multiproduct processes. The implementation of this approach has shown that the optimal sequences of production obtained from the integrated method are more economically attractive than those obtained from a sequential approach. Case studies will be used in this presentation to demonstrate the benefits of the proposed approaches.