Automated Optimization and Control of Modular Chemical Systems

by

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Abstract

Continuous manufacturing has been widely used in many industries such as food, oil, and gas. The pharmaceutical sector has recently begun the transition from batch to continuous manufacturing to leverage potential benefits such as reduction of supply chain disruption effects, production time, drug costs, waste, product quality variations, and improved responses to demand changes. Continuous pharmaceutical manufacturing in compact modular systems provides additional flexibility in where and when the drug is produced.

The transition to continuous operation raises new control challenges to maintain critical quality attributes (CQAs). Process models, facilitated by the widespread adoption of process analytical technology for on-line CQA measurements, enable the concise formulation of existing process understanding and promote real-time decision making and retrospective analyses of the process of interest. First-principles or data-driven models can be developed depending on the degree of process understanding and the purpose for the model construction. Models can be used in process optimization to improve experimental design and manufacturing practices. Models are also used in model-based control. Process control handles variations which would lead to reduced product quality and offers opportunities for bringing processes a step closer towards full automation.

This thesis employs, enhances, and develops modern system engineering tools to address challenges associated with automating optimization and control solutions for modular chemical systems.

First, the thesis presents first-principles mathematical descriptions for common modules in a modular chemical system. An approach is developed for the derivation of linear input-output (step response) models that reduce model-plant mismatch and allow for the successful implementation of a variation of linear model predictive control (MPC), known as quadratic dynamic matrix control. Dynamic optimization for startup based on a first-principles plant-wide model is formulated and solved for a virtual plant for the upstream synthesis of atropine.

Then the thesis presents a methodology for designing stabilizing dynamic state feedback controllers and observers with guaranteed properties for dynamic artificial neural network (DANN) models using matrix inequalities. Assuming a known DANN structure describing a system, a more conservative representation known as a diagonal norm-bounded linear differential inclusion is employed to derive sufficient criteria for estimation and control in the form of linear or bilinear matrix inequality problems using quadratic Lyapunov functions. A computational case study demonstrates the applicability of the method in a realistic multiple-input multiple-output pH control problem.

Lastly, the thesis presents a strategy for constructing nonlinear interpretable input-output models for modules of modular chemical systems. Polynomial nonlinear-autoregressive-with-exogenous-inputs models are identified using a machine learning algorithm that promotes variable selection, grouping of correlated variables, and results in a sparse representation. The models are incorporated in a nonlinear MPC algorithm implemented in the JuMP algebraic modeling language allowing for very fast computational times. Computational case studies of two different chemical reactors demonstrate the successful applicability of the methodology in commonly used modules of modular chemical systems.

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