Process Systems Engineering

Process Control

KEYWORDS: Advanced process control / Regulatory control / Model predictive control / Cyclic adsorption

This research makes significant contributions to the control and optimization of cyclic adsorption processes, particularly in Simulated Moving Bed (SMB) and Pressure Swing Adsorption (PSA) systems. A novel strategy was developed to identify transfer functions in SMB units, enabling the application of classical linear model predictive control (MPC) based on these functions. This approach also addresses the challenges of applying traditional MPC or PID controllers, introducing a modified MPC prediction strategy with a switching system for better handling of dynamic behaviors, and allowing simultaneous control of purity and recovery in True Moving Bed units. Despite the potential superiority of non-linear model-based predictive control (NMPC) over linear MPC, NMPC's practical implementation faces hurdles due to its complexity and computational demands. This work also introduces a nominally stabilizing MPC, or infinite horizon model predictive control (IHMPC), for SMB systems, a significant advancement given the lack of prior research in this area. Additionally, for PSA processes, a new approach was proposed for the simultaneous control and optimization of these systems, addressing the gaps in current literature regarding economic performance tracking and aiming for feasibility in real-time application scenarios. This comprehensive approach enhances the effectiveness and economic efficiency of cyclic adsorption processes, setting a foundation for future advancements in this field.

Introduction

Controlling cyclic adsorption units is complex, especially when integrating control and optimization for economic performance using advanced methods. The challenge arises from dynamic and nonlinear nature, reaching a cyclic steady state, and the interaction among process variables, governed by partial differential-algebraic equations.

The majority of works in cyclic adsorption control use the purities as controlled variables in a linear Model Predictive Control (MPC) setting. Moreover, very few make direct use of process operating variables as direct manipulated variables. Furthermore, only a few works simultaneously controlled the purity and recovery. Finally, the identification of the transfer functions of the processes in study was not found in the literature. As a first contribution to this research line, we presented the development of a novel strategy to identify transfer functions of Simulated Moving Bed units, which makes possible the application of classical linear model predictive controllers based on transfer functions to control these processes. Applying traditional MPC or PID controllers under optimal conditions in the True Moving Bed unit renders the control problem infeasible. To address this, a modified MPC prediction strategy is introduced, utilizing a switching system that selects the most suitable transfer function to manage the unit's unique dynamic behavior. Additionally, this approach proposes simultaneous control of both purity and recovery in the TMB unit.

Several studies in the literature have explored linear model predictive control (MPC) strategies in cyclic adsorption systems whereas non-linear model-based predictive control (NMPC) applications are comparatively less common. Simulations indicate that NMPC strategies outperform linear MPC approaches. However, NMPC's practical implementation is not yet sufficiently developed for widespread use. This is due to a lack of systematic methods for tuning controller parameters, stringent conditions required for stability and feasibility in the closed-loop system, and issues with NMPC convergence when integrated with state estimators. Additionally, NMPC strategies that utilize first principle models often lead to significant computational demands. NMPC strategies potentially outperform linear MPC but require extensive model tuning and parameter adjustments. Stabilizing NMPC often relies on a dual-mode approach with invariant terminal sets, which is computationally intensive. In contrast, linear MPC demands less computational effort, making it more feasible for practical use. This work aims to assess the effectiveness of a stabilizing linear MPC in addressing the limitations of conventional linear MPC in SMB units.

To date, there appears to be no research on using MPC techniques with assured closed-loop stability in SMB chromatography systems. Therefore, as another contribution from our group, we developed and applied a nominally stabilizing MPC controller, also referred to as infinite horizon model predictive control (IHMPC), for controlling the separation of bi-naphthol enantiomers in an SMB process.

Pressure Swing Adsorption (PSA) is another type of cyclic process where automatic control is extremely difficult, especially when integrating control and optimization for economic performance using advanced methods. The main challenge in designing these advanced control and optimization strategies is the intricate dynamics of PSA processes. It is possible to find in the literature some works concerning the application of MPC strategies in PSA units. In the literature, there are studies on the application of MPC strategies in PSA units, but these typically lack integration and do not consider Real-Time Optimization-like economic terms. In this way, there are gaps in the literature to be fulfilled concerning issues associated with PSA process economic tracking. Another contribution from our group is a new approach in the field of PSA operation since up to date there were no reports found in the literature addressing the simultaneous control and optimization of PSA processes. It seeks to develop a strategy feasible to be applied in a real-time scenario, given that using the typical phenomenological model of PSA units internally into an Economic MPC strategy, resulting in non-convex and complex nonlinear programming, is still unfeasible in terms of obtaining the optimal solution within the controller sampling time.

Main Results

Concerning the first contribution, i.e., a novel strategy to identify transfer functions of Simulated Moving Bed units with a modified MPC prediction strategy, several important results were obtained. First, the set of manipulated variables was identified by the orthogonalization method as shown in Table 1. At the non-optimal point, three transfer function matrices linking manipulated and controlled variables were identified: two using the proposed method (GGnon-opt) and one from the full process reaction curve (GRC). This comparison aimed to evaluate the consistency of the proposed method. Additionally, the method was applied to the process under optimal conditions, resulting in two more transfer function matrices (GGopt). Figure 1 presents an example of the models' identification using process data that were generated through a sequence of two 10% increase and two 10% decrease step changes in all manipulated variables, simulated at the optimal point.

Table 1. Identification of manipulated variables: Results obtained from the orthogonalization analysis.

	Operating Variables						
Iteration	Q_S	Q_{IV}	Q_X	Q_E	Q_F	$C_{f,A}$	$C_{f,B}$
1	2.63x10^6	9.79Ex10^6	2.3810^6	5.10Ex10^6	8.0110^3	1.85x10^3	1.93x10^2
2	8.41x10^4	0	3.72x10^5	3.11x10^5	1.71x10^3	1.60x10^3	1.35x10^2
3	2.17x10^4	0	0	1.41x10^5	1.51x10^3	8.88x10^2	1.18x10^2
4	1.27x10^4	0	0	0	2.43x10^2	2.67x10^2	7.52x10^1
5	0	0	0	0	1.51x10^2	2.44x10^2	7.52x10^1
6	0	0	0	0	4.32x10^1	0	5.35x10^1
7	0	0	0	0	3.85x10^1	0	0
8	0	0	0	0	0	0	0

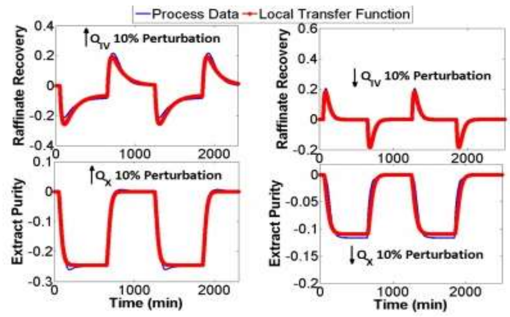

Figure 1. Local Transfer Function Identification for the responses in recovery and purity to step perturbations in recycling and extract flow rates respectively.

Regarding the stabilizing MPC controller for SMB units, we addressed a critical gap in the field to enhance industrial operation. The controller's performance was assessed against a conventional MPC through tests focusing on disturbance rejection and output tracking in scenarios with nonlinear plant-model mismatch. Results showed that while conventional MPC effectively manages the process under design conditions, the proposed IHMPC controller excels both at design conditions and in varied operational scenarios. The IHMPC's superiority, attributed to its infinite prediction horizon, offers improved robustness against plant-model mismatch and maintains process stability amidst persistent disturbances. Figure 2 illustrates the controlled and manipulated variables for the application of the IHMPC controller in the SMB plant.

Regarding the simultaneous control and optimization of PSA processes, a software-in-the-loop environment was used. The virtual plant was controlled by the proposed MPC controller using a Deep Learning model to predict the behavior of the PSA unit over the prediction horizon. The virtual plant was run until reaching its cyclic steady state, and then the controller was activated; Figure 3 presents a diagram of this simulation scheme.

Future Perspectives

Future research in controlling cyclic adsorption processes, such as the Simulated Moving Bed (SMB), could concentrate on developing a robustly stabilizing Infinite Horizon Model Predictive Control (IHMPC). This approach could also be adapted for reactive SMB systems, where the added reaction component introduces further complexity. Additionally, a significant advancement would be to apply these control strategies in a real laboratory-scale unit. This implementation would allow for an empirical evaluation of the effectiveness and performance of the proposed control methodologies. Furthermore, integrating advanced sensing and real-time data

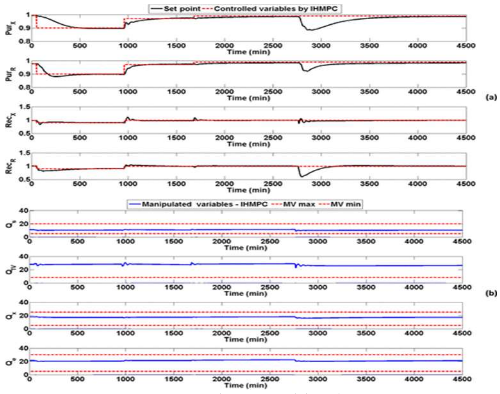

Figure 2. Local Transfer Function Identification for the responses in recovery and purity to step perturbations in recycling and extract flow rates respectively.

analysis could enhance the responsiveness and accuracy of the control systems. Exploring the integration of machine learning algorithms to predict system behavior under varying conditions could also be a valuable avenue for research. This could lead to more adaptive and efficient control strategies, potentially opening up new possibilities in process optimization and efficiency.

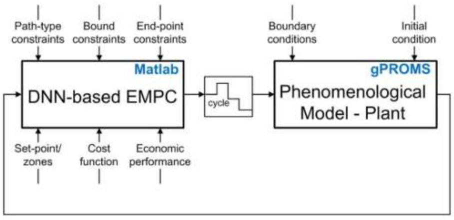

Figure 3. Software-in-the-loop simulation diagramrates respectively.

Related Sustainable Development Goals

Outputs

Master Dissertations

[1] Vinicius Viena Santana, Dynamics of Simulated Moving Bed Reactor Units: Synthesis of N-Propyl Propionate and Transient Analysis, Universidade Federal da Bahia, 2019.

Selected Publications

[1]. I. B. R. Nogueira *et al.*, Computers & Chemical Engineering 133, 106664 (2020)

[2] I. B. R. Nogueira *et al.*, Ind. Eng. Chem. Res. 59, 1979–1988 (2020)

[3] V. V. Santana *et al.*, Computers & Chemical Engineering 137, 106820 (2020).

[4] P. H. M. Oliveira *et al.*, IFAC-PapersOnLine 54, 219-224 (2021).

[5] V. V. Santana *et al.*, Ind. Eng. Chem. Res 60, 4060–4071 (2021).

[6] M. A. F. Martins *et al.*, Separation and Purification Technology 276, 119333 (2021).

[7] T. P. G. Mendes *et al.*, Expert Systems with Applications 210, 118369 (2022)

[8] P. H. M. Oliveira *et al.*, Applied Soft Computing 116, 108318 (2022).

[9] M. A. F. Martins *et al.*, Separation and Purification Technology 306, 122668 (2023).

Team

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