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A centralized/decentralized control approach for periodic systems with application to chromatographic separation processes

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Abstract: In this work we demonstrate the application of our recently presented PAROC framework and software platform for the development of a centralized/decentralized control strategy for the twin-column Multicolumn Solvent Gradient Purification Process (MCSGP) based on multi-parametric control policies. The derived controllers are tested under the presence of disturbances, while their stability is also assessed. The proposed control approach is evaluated under an in-silico, 'closed-loop' fashion against the process model. The designed controller captures efficiently the process setpoints, assuring optimal and stable operation during continuous mode.

Keywords: multi-parametric MPC, control, periodic systems, stability, continuous processing

1. INTRODUCTION

The optimization and control of periodic systems has been discussed extensively in the open literature, resulting to the development of different strategies and methodologies (Nilchan and Pantelides, 1998, Klatt et al., 2000, Kawajiri and Biegler, 2006, Grossmann et al., 2010, Khajuria and Pistikopoulos, 2011, Khajuria and Pistikopoulos, 2013). Such systems are usually associated with highly nonlinear models of large equation sets, the simulation of which requires increased computational force. In particular systems that consider additional domains (e.g. spatial) require special handling that involves domain discretization. The latter can lead to an excessive number of equations, challenging optimization and control studies. Moreover, their periodic nature poses an extra challenge to the design of a holistic control concept and the controller stability, as these systems are characterized by *cyclic* steady state (CSS) (Nilchan and Pantelides, 1998, Huang et al., 2011, Huang et al., 2012). In order for the latter to be established, a cyclic input profile is required that will drive the system to the desired state.

The design and solution of control problems linked to such systems, involve computationally demanding simulations that are often impossible to perform online using current solvers. However, the ability of multi-parametric Model Predictive Control (mp-MPC) to solve the optimization problem *offline* decreases significantly the computational effort required online and allows the solution of more complex problems (Pistikopoulos et al., 2002, Pistikopoulos et al., 2015).

In this work, we present an advanced control strategy of an industrial chromatographic separation process, the Multicolumn Countercurrent Purification Process (MCSGP). MCSGP is a semi-continuous, periodic, chromatographic separation process, used for the purification of various biomolecules (Aumann and Morbidelli, 2007). The control of MCSGP has been visited in several works (Grossmann et al., 2010, Krättli et al., 2011, Krättli et al., 2013), however, here we present a centralized/decentralized approach tracking the output integral leading to periodic input profiles and ensuring CSS. The design, solution and testing of the developed controllers is realized through the application of the PAROC framework and software platform (Pistikopoulos et al., 2015).

2. THEORETICAL BACKGROUND

2.1 The Process

MCSGP is an industrial, ion-exchange, chromatographic separation process used for the purification of various biomolecules. The process separates the mixture in weak impurities (W), product (P) and strong impurities (S). The setup comprises two, identical (i.e. same in physical properties and technical characteristics), ion-exchange, chromatographic columns, operating in countercurrent mode (Figure 1). The columns operate in a semi-continuous fashion, alternating between batch (B-) and interconnected (I-) state. At the beginning of the I1 phase, column 2 starts empty and equilibrated. During this step, the outlet flow of column 1 enters column 2 mixed with an additional fraction of adsorbing eluent (E). This helps the recycling of the impure fraction of the weak impurities and the product. After the completion of I1, the two columns enter B1 phase, where the feed (F) is introduced to column 2 and the product is eluted from column 1. In I2 phase the recycling stream containing the impure fraction of product and strong

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impurities exits column 1 and enters column 2. By the end of I2 phase, column 2 starts eluting pure W (B2 phase). B2 phase finishes when the overlapping region of W and P reach the end of column 2. At this point the two columns switch positions. Therefore, column 1 will go through the recycling and feeding tasks as described above, while column 2 will continue with the gradient elution (Aumann and Morbidelli, 2007, Müller-Späth et al., 2008). The development of advanced optimization and control policies for this process is mainly focused on the maximization of product purity and recovery yield.

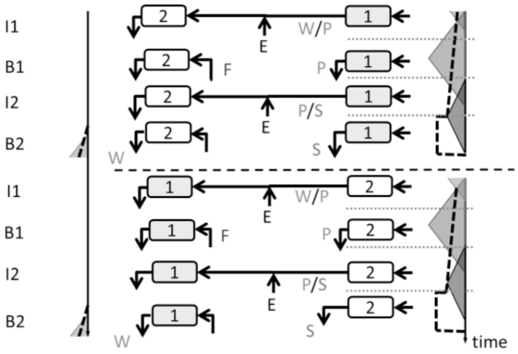

Fig. 1. The twin-column MCSGP (Krättli et al., 2013).

2.2 The PAROC Framework and Software Platform

For the development of the mp-MPC controllers, we follow the PAROC framework and software platform that can be seamlessly applied to a variety of process systems for the development of advanced mp-MPC controllers. In particular, the framework allows in-silico validation of the designed controllers against the original process model, easing their performance evaluation. Fig. 2 illustrates the steps of the framework that consider: (i) process model development, (ii) model approximation/reduction, (iii) formulation and solution of the mp-programming problem and (iv) the in-silico, 'closed-loop' validation. For more details regarding the PAROC framework/software platform the reader is referred to Pistikopoulos et al. (2015).

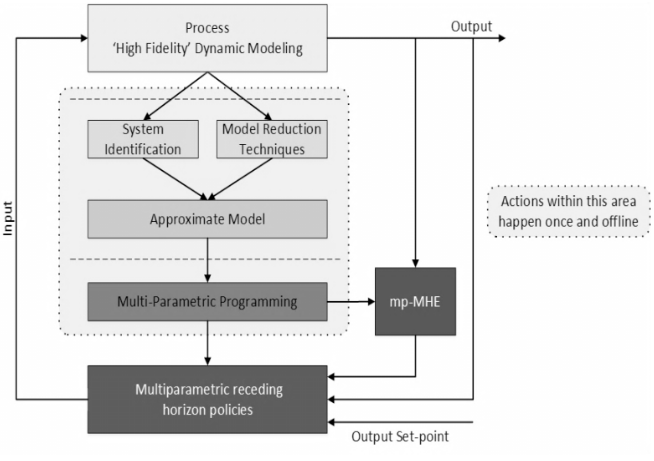

Fig. 2. The PAROC Framework (Pistikopoulos et al., 2015).

2.3 Decentralized control approach during batch operation-Single-column representation

In our previously presented work (Papathanasiou et al., 2015) we develop of a decentralized control strategy for the batch operation of the system. In particular, we decompose the system into two identical sub-systems, for which the mp-MPC controllers are designed and tested. Given the input plethora (modifier concentration, flow rate, feed stream) the system is examined under a random input strategy and the impact of the inputs on the outputs is evaluated. As a result, the flow rate is excluded from the input set as it has no significant impact on the values of the outputs. Additionally, the composition of the stream is uncontrollable as it results directly from the upstream processing and is therefore treated as measured disturbance with experimentally defined variation range. Subsequently, the system considers the modifier as the sole and most significant input, the composition of the feed stream as measured disturbance and the outlet concentrations of the column components as outputs.

As mentioned above, the objective of the separation is to obtain highly pure product at a sufficiently high recovery rate. Grossmann et al. (2010) suggested the calculation of purity and recovery yield using the average concentrations over the process cycle (see (1) and (2)).

$$Pur_{avg} = c_{avp_s,j} \Big/ \left(c_{avW_s,j} + c_{avp_s,j} + c_{avS_s,j} \right) \qquad (1)$$

$$Yj = c_{avp_s,j} \Big/ c_{feed\,p} \qquad (2)$$

where Pur_{avg} and Y_j correspond to the average purity and recovery yield over a process cycle, $c_{avs,j}$ is the average concentration of the mixture components at the end of each cycle, $c_{feed\,p}$ indicates the feed concentration of the targeted product, j indicates the cycle index and s the outlet stream.

Given the above presented equations and aiming to derive a control strategy that will allow continuous process monitoring, we track the integral of the outlet concentrations of the mixture components. In this fashion we can also seamlessly post-calculate purity and yield that define the efficiency of the process. Additionally, since the integral is a continuous function of time it allows tighter process monitoring in comparison to 'cycle-to-cycle' control that monitors discrete outputs.

2.4 Twin-column control concept

In our previous work (Papathanasiou et al., 2015) we focused on the development of decentralized mp-MPC policies that are able to monitor the two columns independently, during batch operation (B- phases). In this work, we extend our methodology to the development of advanced centralized/decentralized control strategies that will effectively ensure optimal operation under continuous mode (interconnected (I-) phases). The decentralized control strategy presented in Section 2.3 is therefore extended for the development of a holistic control concept, where the system