Online 'cycle to cycle' optimizing control of Varicol and Simulated Moving Bed (SMB) processes

Mohammad Amanullah[1], Cristian Grossmann[2], , Marco Mazzotti[1,]*, Manfred Morari[2], Massimo Morbidelli[3]

[1] *Institute of Process Engineering, ETH Zurich, CH-8092 Zurich, Switzerland*

[2]*Automatic Control Laboratory, ETH Zurich, CH-8092 Zurich, Switzerland*

[3] *Institute for Chemical and Bio-Engineering, ETH Zurich, CH-8093, Switzerland*

* Corresponding author: marco.mazzotti@ipe.mavt.ethz.ch

Simulated Moving Bed (SMB) and Varicol are well established technologies for continuous chromatographic separation especially for enantiomers[1]. However, optimum SMB or Varicol operation is a challenge and currently these processes are operated sub-optimally to ensure robustness. Consequently, control and automation of SMB is receiving increasing attention lately to exploit the full economic potential of these processes[2-8]. These control schemes require accurate physical data i.e., adsorption isotherm, column voidage, and dispersion parameters' which are difficult to measure, time consuming and may change over time due to aging of the stationary phase.

On the other hand, the control group at ETH Zurich has developed an SMB control scheme which guarantees the fulfillment of product and process specifications and optimizes the economics of process at the same time. Besides, this controller requires only minimal information such as adsorption behavior at infinite dilution and average void fraction of the columns. A summary of the papers dealing with this control scheme are elaborated here. In our first paper, we developed a new optimization-based control strategy. A linearized time-varying reduced-order model that accounts for the periodic nature of the SMB process has been used for on-line optimization and control of SMBs[9]. Four internal flow rates, which can be adjusted via external flow rates, have been used as the manipulated variables. On-line concentration measurements at the product outlets together with a periodic Kalman filter are used to reduce the effect of model errors. Optimal input adjustments that allow for the achievement of process specifications and optimal performance are calculated on the basis of the predicted evolution of the plant. The realization and implementation of the concept on a virtual eight-column SMB unit is described, and the capability of the controller to run the SMB plant at its economic optimum regardless of possible disturbances and model uncertainties is assessed.

In the second publication, we had presented the implementation of this concept on a virtual eight column SMB platform in the case of binary linear systems through simulation[10]. For a whole series of typical plant disturbances, it has been shown that the proposed approach is effective in minimizing off-spec products and in achieving optimal SMB operation, also in the case where there are significant model uncertainties.

In the third paper, we had presented the controller's performance, through simulation studies, for a system characterized by non-linear adsorption isotherm[11]. This paper illustrated how a controller that is based only on the linear adsorption isotherm parameters can find the correct operating conditions for the SMB applied to a system characterized by a nonlinear competitive isotherm in order first to fulfill the product specifications and then to optimize the economics of the operation. The performance of the controller was assessed for several scenarios addressing the main challenges in SMB operation.

A further assessment of the controller was presented in the fourth paper which focused on the implementation of the control concept to SMBs operating under overloaded chromatographic conditions that are characterized by nonlinear competitive adsorption isotherms[12]. It has been shown that despite the overloaded chromatographic conditions, the process can be controlled and optimized based on the linear adsorption isotherm information only. The performance and robustness of the control scheme is assessed under simulated challenging operating conditions.

Experimental implementation of this control concept on a laboratory scale 8 column SMB unit, for the separation of a mixture of Uridine and Guanosine characterized by linear adsorption isotherm, is presented in the papers from fifth through seventh[13-15]. In the fifth paper the goal was two-fold[13]. Firstly, to experimentally evaluate and demonstrate the capability of the controller to optimize and operate the SMB units, thus delivering the products with maximum productivity and minimum solvent consumption. Secondly, to show the suitability of the controller even using a minimum of system information, thus making the detailed isotherm measurements redundant and saving time in the separation design phase. Further results, demonstrating the experimental implementation of this control concept were presented in the sixth paper[14]. On the seventh paper, the performance of the SMB control scheme was demonstrated via several experimental controlled SMB runs that were designed to challenge the robust performance of the controller[15]. The reported results have demonstrated that the controller is able to deliver the products with the specified purities and to optimize the process performance despite uncertainties in the system behavior and disturbances taking place during the operation.

The controller described above, was based on continuous online monitoring and frequent controlling (64 times in a cycle) of the SMB unit. However, accurate online monitoring of the SMB unit is a key challenge for the efficient implementation of any control scheme especially for chiral systems due to a number of technical and system specific constraints and presence of impurities. A more pragmatic approach would be to develop a control scheme that makes use of existing and accurate monitoring schemes currently used in the industry such as HPLC analysis over every cycle ('cycle to cycle'). However, this imposes additional loads on the controller since it gets less frequent information, i.e. once in a cycle, from the plant to take necessary control actions. Therefore, evaluation of the performance of this optimizing controller under 'cycle to cycle' information is important for implementing it to industry and reaping the full economic benefits of this.

This work reports experimental validation of the 'cycle to cycle' control scheme in a laboratory scale SMB unit for the separation of a binary mixture of nucleosides exhibiting linear isotherm. The effectiveness of the 'cycle to cycle' control scheme is also shown by several simulations of SMB and Varicol processes under nonlinear chromatographic conditions. The results illustrate that the 'cycle to cycle' controller is able to meet the products' purity specifications and operate the process optimally with minimal information regardless of the disturbances that might take place during the operation. Besides, we also envisage presenting results of experimental implementation of the 'cycle to cycle' controller for the separation of a chiral compound in a laboratory SMB unit.

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