NONLINEAR MODEL PREDICTIVE CONTROL OF A SIMULATED MOVING BED UNIT

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ABSTRACT – The simulated moving bed (SMB) is a type of continuous chromatographic separation, formed by a train of chromatographic columns. Operating a SMB unit is a complex task due to its low operating range and its sensitivity to any change. In order to control the system in an efficient way, a rigorous model with a suitable computational strategy was employed in this work. The polynomial approximation method in finite element was used to discretize the spatial variable of the internal model of a NMPC controller. The satisfactory performance of the controller, when applied to separate the enantiomers of praziquantel subject to equipment failures, was achieved within an acceptable computational effort for real-time application.

1. INTRODUCTION

The simulated moving bed (SMB) is a chromatographic separation technique that has gain great interest in fine chemicals and pharmaceutical industry (Hjorth et al., 2008). This process can generate high productivity with low eluent consumption (Zhang et al., 2003). The separation of enantiomers into chiral compounds is one of the most important applications of SMB (Rajendran et al., 2009). In order to optimize and control a SMB in an efficient way, rigorous models with good computational strategies are desired (Rajendran et al., 2009). It has recently been shown that for mixtures with simpler absorption isotherms such as linear or Langmuir type, it is possible to use nonlinear predictive control (Andrade Neto et al., 2016).

In this work the SMB was approached with polynomial approximation in finite elements (PAFE). The performance of PAFE approximation was compared with finite differences and evaluated within a nonlinear model predictive controller of a SMB unit. In this case, a failure test of the switching valve was analyzed.

2. MATHEMATICAL MODEL

The basis of the mathematical model for the SMB is the fixed bed model of the adsorption columns, which is well established (Shafeeyan et al., 2014). The mass balance for the \( i \)-th component in the \( k \)-th column is given by:

\[
\frac{\partial C_{i,k}}{\partial t} = -v_{m,k} \frac{\partial C_{i,k}}{\partial z} + D_{i,k} \frac{\partial^2 C_{i,k}}{\partial z^2} - \left( \frac{1-\varepsilon_k}{\varepsilon_k} \right) \frac{\partial q_{i,k}}{\partial t}
\]

with the follow initial and boundary conditions:
\[ C_{i,k}(0,z) = C_{0,i,k}(z) \]  
(2)

\[ D_{i,k} \frac{\partial C_{i,k}}{\partial z} \bigg|_{z=0} = v_m,k \left[ C_{i,k}(t,0) - C^i(t) \right] \]  
(3)

\[ \frac{\partial C_{i,k}(t,z)}{\partial z} \bigg|_{z=d_i} = 0 \]  
(4)

in which the subscript \( i \) corresponds to the components A or B; \( k = 1,2,\ldots,N \), system columns; \( C[M L^{-3}] \) is the mass concentration in the fluid phase; \( t[T] \), the time; \( v_m[LT^{-1}] \), the effective velocity; \( z[L] \), the axial coordinate; \( \varepsilon \), the overall bed void fraction; \( D[L^2T^{-1}] \), the effective dispersion coefficient; \( q[M L^{-3}] \), the mass concentration of the adsorbed phase; \( C_0 \), the initial concentration at \( t = 0 \), \( C^i(t) \), the column inlet concentration with the superscript \( j = I, II, III, IV \) counting over the sections; and \( l[L] \), the column length. The instantaneous equilibrium between the stationary and mobile phase was assumed, and a linear isotherm was used. It was presumed that the SMB operates in a classical manner, where all stream advance in a synchronized way with a constant switching time \( \theta \).

3. OPTIMIZATION AND CONTROL

The cyclic stationary regime of the SMB, where the concentration changes periodically in all positions of the unit, particularly in the port of extract and raffinate, was optimized. The reduced feasible region of operation in the SMB is delimited by the triangle theory (Rajendran et al., 2009). The best operation point can be find optimizing the internal flows \( (Q) \) within the feasible region in the SMB. The objective function used in the optimization problem maximizes raffinate and extract productivity and minimizes solvent consumption, and was the same used in the controller, expressed as follows:

\[
J = \left( Q_d \left< C_{x,d} \right> + Q_e \left< C_{r,e} \right> - Q_x \right) W_1 - \left[ \left( P_{x,min} - \left< P_x \right> \right)^2 + \left( P_{r,min} - \left< P_r \right> \right)^2 \right] W_2
\]  
(5)

where \( \left< C_{x,d} \right> \) and \( \left< C_{r,e} \right> \) are the steady-state mean concentrations; \( Q_d \), \( Q_x \), \( Q_e \) are the solvent, extract and raffinate flow rates; \( \left< P_r \right> \) is the steady-state purity; \( P_{r,min} \), the minimum acceptable purity value; \( W_1 \) and \( W_2 \) are weighting factors. In the control algorithm, the model equations are integrated starting from the current state of the plant, which is assumed to be known from on-line measurements, to the prediction horizon, \( H_p \). The calculated control actions are the internal flows in the sections of the SMB unit, that can easily be converted in terms of the external flows.

3. RESULTS

To evaluate the polynomial approximation in finite elements method for optimization and control, the separation of the enantiomers of praziquantel was considered.
3.1 Spatial Derivative Approximation

Column and equilibrium parameters for praziquantel were provided by (Coelho et al., 2017).

Table 1 – Parameters for praziquantel separation. The index A refers to the less retained enantiomer; B the more retained; r, the raffinate; x, the extract.

| Parameters     | Value   | Parameters     | Value   | Parameters     | Value   |
|----------------|---------|----------------|---------|----------------|---------|
| $l (cm)$       | 10      | $D_B (cm^2 min^{-1})$ | 1.265   | $Q_B (cm^3 min^{-1})$ | 6.234   |
| $d (cm)$       | 1       | $C_{f,A-B} (g \cdot L^{-1})$ | 1       | $Q_{II} (cm^3 min^{-1})$ | 9.893   |
| $\epsilon$    | 0.742   | $\theta (min)$ | 2.5     | $Q_{III} (cm^3 min^{-1})$ | 5.645   |
| $D_A (cm^2 min^{-1})$ | 1.169   | $Q_{I} (cm^3 min^{-1})$ | 10.707  | $P_{r,x} (%)$ | 99      |

In order to determine the mesh size, different discretization was made in both PAFE method and in finite difference method. In the PAFE, one and two finite elements were used, and the results are shown in Figure 1.

![Figure 1](image)

Figure 1 – Separation profile of praziquantel. a) Internal points for polynomial approximation. b) Internal points for finite differences.

Based on Figure 1, it is observed that for the case of polynomial approximation (Figure 1a) a much smaller mesh of discretization with respect to finite differences (Figure 1b) is needed to describe the system. The global polynomial approximation (1 FE) may not be appropriate in regions where the system response has flat behaviors. In this case, PAFE may be a better option with a higher number of finite elements and fewer internal points. In the control study, two finite elements and 11 internal points were used.

3.2 Control

A NMPC study was performed on the SMB considering a malfunction in the switching valve. A prediction horizon used in the control was $H_p = 1$ cycle, which is equivalent to 8 sampling periods. A disturbance of -25% of initial value of the switching valve time was applied after the first cycle and is shown in Figure 2.

For the system without any control action, the disturbance affects the purity of the
extract and raffinate, crossing the minimum limit of 99% defined in the setpoint (see Figure 2a). When the control action is activated, the NMPC responds to the disturbance and drives the variables back to the setpoint, as seen in Figure 2b. In the all operation time, the difference between the sampling time (switching time) with the computational time spent to calculate the control actions were positive, which makes NMPC feasible for real-time application.

4. CONCLUSIONS

The polynomial approximation required much smaller discretization mesh than finite difference in the SMB model. The NMPC response to the failure of switching valve was carried out for praziquantel separation, using two finite elements and 11 internal points, and the controller was able to keep the variables controlled in the desired values with computational effort within the allowed limit.

5. REFERENCES

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