Modeling of Simulating Moving Bed Process

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An SMB system consists of multiple columns connected to each other making a circulation loop (Fig. 1). SMB system consists of four zones, each fulfilling different functions. The feed and desorbent are supplied continuously through the inlet ports and at the same time extract and raffinate are withdrawn at the outlet ports. These four inlet/outlet ports are switched in the direction of liquid flow at a regular interval, T. The same switching operation is repeated for N_{col} steps which constitutes a cycle. Since SMB repeats the same operation for number of columns, this symmetric operation can be exploited to reduce the problem size by a single-step optimization formulation [1]. Here, operation is considered over only one step where the profiles at the beginning of a step are identical to those of the downstream adjacent column at the end of the step which ensures a CSS condition at the end of a cycle.

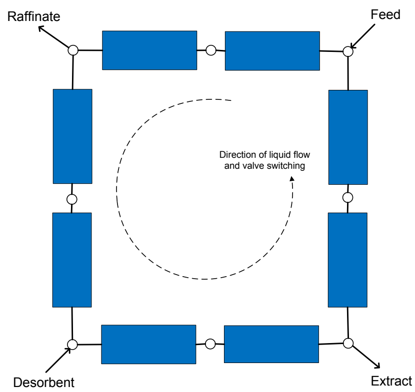

Figure 1: SMB Process

The behavior of the chromatographic columns, identified by index $n = 1 \dots N_{col}$ is described through an equilibrium assumption between the solid and liquid phases along with a simple spatial discretization. Here, the mass balance in the liquid phase is given by,

$$\epsilon_B \frac{\partial C_{n,i}(x,t)}{\partial t} + (1-\epsilon_B)\frac{\partial q_{n,i}(x,t)}{\partial t} + \frac{Q_n(t)}{S_n}\frac{\partial C_{n,i}(x,t)}{\partial x} = 0 \qquad i = A, B \tag{1}$$

The equilibrium relationship between the solid and liquid phases is given by,

$$\frac{\partial q_{n,i}(x,t)}{\partial t} = K_i(C_{n,i})C_{n,i}(x,t) \tag{2}$$

where, $C_{n,i}$ is the concentration of component i in column n in the liquid phase; $q_{n,i}$ is the concentration of component i in column n in the solid phase; Q_n is the volumetric flow rate in each zone n; S is the cross-sectional area of the bed and ϵ_B is the bed voidage. We assume that the zone velocities are constant during a step and all the inlet/outlet ports are switched simultaneously. Dividing the column into N_{dis} compartments and applying a simple backward difference results in,

$$\frac{dC_{n,i,j}}{dt} = K_i(C_{n,i,j})N_{dis}Q_n[C_{n,i,j-1} - C_{n,i,j}] \tag{3}$$

for $j = 1 \ldots N_{dis}$; $i = A, B$ (binary mixture); $n = 1 \ldots 6$. We define the state variables for this system, $C_{n,i,j} = x_m(t), m = 1 \ldots 12N_{dis}$ as the concentrations of A and B in the jth compartment for the six columns where the index is ordered as: $m = j + (n-1)N_{dis}$ for component A and $m = j + 6N_{dis} + (n-1)N_{dis}$ for component B.

The SMB system considered in the AMPL file is divided into four zones each of which consist of $n_I = 1, n_{II} = 2, n_{III} = 3, n_{IV} = 4$ columns. The compartments are numbered $i = 0, ..., (n_I + n_{II} + n_{III} + n_{IV})N_{dis} - 1$. The port switching time, T and the constant flows, $q = [Q_I, Q_{De}, Q_{Ex}, Q_{Fe}]^T$ as independent decision variables while the remaining flows $Q_{II}, Q_{III}, Q_{IV}, Q_{Ra}$ are determined from a linear mass balance. In this case study, we consider the linear adsorption isotherm: $K_A = 2, K_B = 1$. The indices of the port locations are defined as,

$$\begin{aligned} n_{Ex} &= n_I N_{dis} \\ n_{Fe} &= (n_I + n_{II})N_{dis} \\ n_{Ra} &= (n_I + n_{II} + n_{III})N_{dis} \\ n_{De} &= (n_I + n_{II} + n_{III} + n_{IV})N_{dis} \end{aligned} \tag{4}$$

Mass balance equations plus additional equations determing the compositions of both components ($i = A, B$) in the raffinate, extract and feed are:

$$\begin{aligned} \dot{C}_{0,i} &= k_i(Q_{IV}C_{n_{De-1},i} - Q_I C_{0,k}) \\ \dot{C}_{j,i} &= k_i Q_I(C_{n_{j-1},i} - C_{j,i}) \quad j = 1..n_{Ex-1} \\ \dot{C}_{j,i} &= k_i Q_{II}(C_{n_{j-1},i} - C_{j,i}) \quad j = n_{Ex}..n_{Fe-1} \\ \dot{C}_{n_{Fe},i} &= k_i(Q_{II}C_{n_{Fe-1},i} + Q_{Fe}C_{n_{Fe},k} - Q_I C_{0,k}) \\ \dot{C}_{j,i} &= k_i Q_{III}(C_{n_{j-1},i} - C_{j,i}) \quad j = n_{Fe+1}..n_{Ra-1} \\ \dot{C}_{j,i} &= k_i Q_{IV}(C_{n_{j-1},i} - C_{j,i}) \quad j = n_{Ra}..n_{De-1} \\ \dot{M}_{Ex,i} &= Q_{Ex}C_{n_{Ex-1},i} \\ \dot{M}_{Ra,i} &= Q_{Ra}C_{n_{Ra-1},i} \\ \dot{M}_{Fe,i} &= Q_{Fe} \end{aligned} \tag{5}$$

The optimization problem considered is to maximize the throughput subject to the dynamic model equations, the CSS conditions and purity constraints. CSS conditions can be formulated as equality constraints,

$$\begin{aligned} x_m(0) - x_{m+N_{dis}}(T) &= 0 \quad m = 1, ...5N_{dis} \\ x_m(0) - x_{m-5N_{dis}}(T) &= 0 \quad m = 5N_{dis} + 1, ...6N_{dis} \end{aligned} \tag{6}$$

0.1 Exact Jacobian evaluation, $A(x_k)$

Given, the state equations, we evaluate the Jacobian

$$A \equiv \nabla C^T = \left[I - \frac{\partial y(t_f)}{\partial y_o} \quad \vdots \quad - \frac{\partial y(t_f)}{\partial p} \right] \tag{7}$$

by using direct sensitivity equations which can be obtained by differentiating the original model equations with respect to the parameters, y_o and p. Define,
$s(t) = \frac{\partial y(t)}{\partial p} \in \mathbb{R}^{ny+np}$

$$\frac{\partial}{\partial p}\{\dot{y} = f(y,p) \quad y(0) = y_0\} \tag{8}$$

results in,
$\dot{s} = f_y s + f_p v \qquad s(0) = Iv$
where

$$v_k = \begin{cases} 1 & if\ k \leq ny \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

and I is an identity matrix of size $(ny + np)$. The sensitivity equations depend on states $y(t)$ and can be solved simultaneously with the state system. The structure of the linear sensitivity equations has been exploited in DAE/ODE solvers by using methods like staggered-corrector techniques.
Since the sensitivities are independent of each other,, the sensitivity calculations can be parallelized. Therefore, a subset of the sensitivities are solved on each processor along with a copy of the state variables. The SMB bed model is solved for CSS using Newton's method. Here, we use the rSQP solver to solve the non-linear system. The necessary function and gradient evaluation is provided by intergrating the differential equations using CVODES and the RHS of the sensitvity equations is provided using automatic differentiation tool, ADOL-C.

References

[1] Y. Kawajiri and L. T. Biegler. Optimization strategies for simulated moving bed and powerfeed processes. AIChE Journal, 52(4):1343 1350, 2006.