A Software Package for the Optimal Operation of Continuous Moving Bed Chromatographic Processes

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Abstract: This software package includes numerical methods for **modeling**, **parameter estimation**, **design** of **experiments** and **optimal** operation of continuous moving bed chromatographic processes. Its application to a production of a high fructose corn syrup in a reactive moving bed process will be demonstrated.

Simulated Moving Bed chromatography (SMB) is an important separation process in industrial production. It consists of 6 to 24 chromatographic columns which are connected in a closed-loop arrangement. A counter-current movement between the solid and the liquid phase is achieved by advancing the inlet and outlet ports *synchronously* or *asynchronously* in direction of the liquid flow. Due to the hybrid and complex dynamic and because of a strong nonlinear adsorption behavior, optimization and control of SMB processes present challenging tasks.

A lot of work has already been published on modeling of chromatographic processes. The *general rate model* is the most rigorous mathematical modeling approach, from which other model versions can be derived by ignoring one or several effects. The resulting PDE systems are solved using a combination of finite element method and orthogonal collocation (Gu, 1994). The estimation of the model parameters is done by least-squares. The identifiability of the parameters, i. e. their division in identifiable groups, as well as the design of new experiments are determined based on the fisher-information matrix (Majer, 1997).

The SMB-process is optimized using a sequential approach based on a rigorous mathematical model of the plant. This problem requires formidable efforts and can not be achieved within a fixed sampling time. On the other hand, disturbances and plant/model mismatch can occur and lead to an off-spec product. In order to maintain the product purity while injecting a minimal additional amount of eluent, we propose a modified nonlinear model predictive controller, where we are calculating a *suboptimal* but *feasible* solution and which can be applied in real-time.

All parts of the package (parameter estimator, experiment designer, optimizer and controller) are programmed in Fortran 90 and can be used as independent programs. In order to combine and use all of them in parallel, a user-friendly graphical interface was written in JAVA. The use of the software will be demonstrated on a reactive SMB process for the production of high fructose corn syrup.

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