117ª DEFESA DE TESE EM ENGENHARIA INDUSTRIAL

PROGRAMA DE PÓS-GRADUAÇÃO EM ENGENHARIA INDUSTRIAL - PEI

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Título: "ENANTIOMERS RESOLUTION IN SIMULATED MOVING BED: PARAMETER ESTIMATION AND UNCERTAINTY ANALYSIS."

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Resumo:

Pairs of enantiomers in pharmaceutical drugs are known to might have one enantiomer with the active principle, whereas the other might cause severe side effects. However, enantioresolution is not trivial. Simulated Moving Bed (SMB) chromatographies have been applied in the industrial and lab scales for separation of enantiomers. A representative phenomenological model is a key to a successful design, optimization, and control of the system, that relies on well-estimated parameters. This thesis aims to propose a novel methodology for a global and straightforward parameter estimation of the SMB model coupled with uncertainty analyses. Firstly, parameters are estimated via gradient-based and Particle Swarm Optimization (PSO) methods, whose operating conditions were generated by Latin Hypercube Sampling (LHS). Then, a new parameter estimation is carried out using experimental data from the literature, together with a PSO population-based uncertainty evaluation that enables model validation and definition of the parameter confidence regions. Secondly, this work proposes a method for screening the adsorption isotherm based on minimal system knowledge. This methodology determines a minimum number of experiments to be carried out in an SMB unit to provide a representative model, followed by a new parameter estimation and screened of the best adsorption isotherm equation. Finally, a single isotherm equation Linear + Bi-Langmuir is introduced as a combination of other known equations in the literature in order to carry out estimability analysis together with a comparison with screened isotherm. An estimability analysis based on orthogonalization could determine a subset of uncorrelated parameters which can be estimated, enabling the reduction of computational effort during parameter estimation. The results of this study show that it is possible to perform parameter estimation from SMB chromatography producing a more trustworthy model with minimal system knowledge for different adsorption isotherm equations that could make parameter estimation faster and then, enantiomer resolution simpler.

Palavras-chaves: Enantiomers, Simulated Moving Bed, Parameter Estimation, Uncertainty Analysis, Sensitivity Analysis.

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