Epidemic Genetic Algorithm for the Solution of an Inverse Mass Transfer Problem

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ABSTRACT

Recent developments in the pharmaceutical industry have led to the discovery of increasingly complex substances, and a large number of drugs going to market at the moment are chiral substances with optical isomers. Even though the physical properties of optical isomers are very similar, their effects on the human organisms may be drastically different, possibly causing harmful side effects.

Therefore, there is a growing demand for efficient methods to purify optical isomers, with one of the most promising alternatives being the simulated moving beds (SMB) chromatography. For the full understanding of the operation of SMBs, and a possible scale-up to industrial production, it is required a better knowledge of the mass transfer mechanisms involved and their dependence on the physico-chemical and process parameters. The first step in that direction consists of the characterization of adsorption columns with the determination of phisico-chemical parameters such as dissociation constant, k_d, and maximum capacity of adsorption of the adsorbent resin, q_m. In the present work the Thomas` model with an analytical solution is used for the solution of the direct problem. The forward model yields good solutions when the axial dispersion coefficient is negligible. The inverse problem is formulated implicitly in which we seek to minimize the norm of the squared residues between calculated and measured values for the breakthrough curves, and for its solution the Epidemic Genetic Algorithm is used.

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