Simulation and optimizing control of continuous annular electro-chromatography (CAEC)

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Capillary electro-chromatography, the combination of capillary electrophoresis and high performance liquid chromatography, is a very efficient separation tool for analytical applications. The transfer to the preparative scale promises to provide a highly efficient separation technology for industrial biotechnology and for the pharmaceutical industry. The concept of annular chromatography additionally enables the operation of electro-chromatography as a continuous process. In this paper, we describe the modeling and dynamic 2D-simulation of the resulting Continuous Annular Electro-Chromatography (CAEC) and investigate an online optimization and control strategy.

In the model, axial and annular dispersion, mass transfer resistances and multi-Langmuir adsorption isotherms are considered. A separation of two compounds is investigated. The exponential high-order compact (EHOC) alternating direction implicit (ADI) method [1] is used to solve the dynamic non linear partial differential equations. The influence of an inhomogeneous, statistically distributed electroosmotic flow (EOF) is investigated.

To maximize the throughput under constraints on product purity and yield, an optimization of the steady-state operating conditions of the CAEC unit is performed. Further, an online optimizing control strategy is proposed in which model mismatch and measurement errors are taken into account. It is based on the iterative gradient-modification set point optimization proposed for batch chromatography in [2].

Keywords: capillary electro chromatography, annular chromatography, CAEC, distributed parameter models, EHOC ADI, iterative set point optimization

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Literature

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