MODELING AND SIMULATION OF FIXED-BED AND SIMULATED MOVING BED CHROMATOGRAPHIC PROCESSES USING PDECOL, EPDCOL, BACOL AND BACOLR SOFTWARE PACKAGES

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ABSTRACT

Modeling and simulation of chemical engineering processes always attracted a special attention since it could lead to significant savings in time and materials. The problem of modeling a simulated moving bed (SMB) separation process can be analyzed by two different strategies: one, by simulating the system directly, as a set of fixed-bed chromatographic columns and taking into account its intermittent behavior; other by representing its operation in terms of a true counter current system. The first model represents the real SMB and considers the periodic switch of the injection and collection points. The second is developed by assuming the equivalence with the ideal true moving bed (TMB), where solid and fluid phases flow in opposite directions [1].

The SMB and TMB models must be numerically solved, using software packages for nonlinear partial differential equations (PDEs) in one space and one time dimension. The objective of this work is to compare related software packages, such as PDECOL [2] and BACOL [3], to solve these kind of separation processes. PDECOL software, still widely used in Chemical Engineering problems, is based on the method of lines and uses a finite element collocation procedure for the discretization of the spatial variable. The collocation procedure reduces the PDE system to an initial-value ODE system, which then depends only on the time variable. BACOL is an adaptive method of lines software package, developed for solving one dimensional parabolic partial differential equations. Contrary to PDECOL, BACOL has the ability to change the number of mesh points and thus control the spatial error. In this way, the remeshing strategy of BACOL software allows it to control both the spatial error and the temporal error. Computational results presented by the authors [4] indicate that BACOL is reliable and extremely efficient in dealing with problems having solutions with rapid variation. The objective of this work is to evaluate the potentiality of this software package to solve SMB chromatographic processes, which are also characterized by moving concentration fronts.

REFERENCES

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