Nonlinear Mathematical Model of Preparative Chromatography

한순구, 최영재, 정성택, 이윤우[1], 김재덕[1], 노경호[*2]
인하대학교 화학공학과; [1]한국과학기술원;
[2]인하대학교 생명화학공학부
(rowkho@inha.ac.kr[*])

Enantiomers have the same physical properties without optical property, and exhibited different activity in human body. One of enantiomer pair has medical activity, and the other shows seriousness side effect. Because of difficult synthesis, separation by LC with CSP has been widely used. In this study, the separation condition for racemic bupivacaine was investigated by mathematical model with competitive Langmuir isotherm to find the optimum feed condition, injection volume and injection concentration.The parameters of competitive Langmuir isotherm were assumed and fitted to the experimental data by solving the mathematical adsorption equations with commercially available gPROMS. For each racemic compound, mass transfer coefficients k were obtained by parameter estimation and maximum likelihood method. The agreement of elution profiles between the experimental data and the calculated values was fairly good. In order to find the optimum separation condition, simulations were carried out to determine the feed conditions. It was experimentally confirmed that for the feed conditions to separate preparatively racemic bupivacaine.