Prediction of the elution profile of aromatic compounds in RP-HPLC

노경호*, 김은철
인하대학교
(rowkho@inha.ac.kr*)

An efficient prediction of the elution method was used to separate aromatic compounds such as benzene, toluene, chlorobenzene, O-xylene, and 1,2-dichlorobenzene by RP-HPLC. In this work, the binary mobile phase of water and methanol was used. The retention time and bandwidth were predicted under linear-gradient condition with the four retention models. The elution profiles were calculated based on the linear and quadratic equations of retention factor, $\ln k = \ln kw + S\varphi$, $\ln k = L + M\varphi + N\varphi 2$, $k = A + B/\varphi$, $k = A/(1 + B\varphi n)$, where φ was the vol.% of methanol. The elution profiles were calculated by the Guassian distribution with obtained retention time and bandwidth. In the experimental conditions, the agreement between the experimental data and the calculated values was relatively good. The experimental and calculated results performed that the first mobile phase composition was water/methanol, 96/4 vol.%, followed at 60, 40, and 20 min later by the second composition of mobile phase which was linearly changed to 24/76 and 40/60 vol.%, respectively. The minimum average error of calculated and experimental results of aromatic compounds of benzene, toluene, chlorobenzene, O-xylene, and 1,2-dichlorobenzene were showed lower than 3.5% by Bi-poly equation.