

Optimized calibration curve for size exclusion chromatography applied to poly(vinyl chloride)

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The problem of using a polystyrene-standard-based calibration curve for other polymers has been overcome by developing an algorithm based on the concept of parameter estimation and optimization. The algorithm modifies the regression coefficients of the polystyrene-standard-based calibration curve by interactively using the chromatographic output and the absolute number-average molecular weight of the experimental polymer. Analytical expressions have been derived for calculating the directional derivatives, which ensure rapid convergence of the objective function. The algorithm, applied to commercial poly(vinyl chloride), offered a number-average molecular weight of 32 037 whereas that measured by membrane osmometry is 32 000. The polymer characterization parameters calculated from the optimized calibration curve closely matched those obtained from the universal calibration curve and Q -factor values. The algorithm needs no narrow standard of the experimental polymer, and holds for homopolymers, copolymers and polymer blends. It can be easily incorporated into commercial size exclusion chromatography data-reduction software packages.

(Keywords: poly(vinyl chloride); size exclusion chromatography; universal calibration)