A study of SEC chromatograms on the basis of polymer structure properties

Size Exclusion Chromatography (SEC), widely used in polymer laboratories, provides a convenient method for the determination of full molecular weight distribution (MWD) of polymers. For linear homogeneous polymer samples, the procedure to estimate the true MWD based on the elution curve of SEC has already been well established, while for nonlinear polymer samples and mixtures of linear and nonlinear polymers, the measured SEC data are often used just qualitatively. The SEC separation process is rather complicated, and a detailed study using finite element method and/or Brownian Dynamics simulation technique is rather difficult without oversimplifying the problem dramatically. However, it has been known for long that SEC separates polymer molecules according to their size in dilute solutions, and experimental studies with well-defined linear and nonlinear polymer samples have shown that a universal curve may exist between the SEC retention volume and polymer structure properties such as hydrodynamic volume, hydrodynamic radius and radius of gyration. Those structure properties can be determined by intrinsic viscosity measurement, dynamic and static light scattering respectively, and the measured values are often certain statistical averages weighted by all the polymers present in the sample. On the other hand, those structure properties and many others can be reasonably estimated by computer simulation techniques such as random walk simulations, self avoiding walk simulations or detailed Monte Carlo simulations. Such calculations can be performed for polymer molecules with almost any kind of chain architectures, and can therefore be formulated into a model in the study of SEC chromatograms of complex polymer samples within the framework of universal calibration strategies. In this study, such a model is formulated and several experimentally obtained SEC chromatographs will be reinvestigated in detail.