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Computer study of the chromatographic separation process: Separation of linear and branched polymer chains

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The general principles of chromatographic separation of mixtures of linear and branched polymers were studied by Monte Carlo simulations. The study focuses on the conditions relevant for experimental chromatography, i.e., on the partitioning of fairly dilute solutions between bulk solution and mildly sterically confined pores. The polymer chains were modeled as self-avoiding walks either in a good or in theta solvent. The partition coefficient of branched chains (K_B) is higher than the partition coefficient of linear chains (K_L) in pores with non-attractive walls and the difference between both coefficients evaluated in mixtures of polymers with different chain architectures exceeds that based on values for single chain systems. However, it decreases with increasing adsorption strength of chains on pore walls, i.e., with increasing attractive interaction between pore walls and polymer structural units, ε. For ε ca. -0.18, the partition coefficients equal ($K_L = K_B$) and later their sequence inverts. Evaluation of concentration profiles and structural characteristics of the chains at different distances from the wall reveals that more deformable linear polymers preferentially accumulate close to the attractive walls and orient parallel with the wall. The study shows that the stationary phase in neat size exclusion chromatography has to be optimized from the physico-chemical point of view, because the separation efficiency can be significantly deteriorated by its improper choice. However, the combination of size exclusion and interaction chromatography can be used for analysis of complex systems (e.g., mixtures of polymers and copolymers) when it is desirable to suppress the separation with respect to some molecular characteristics and separate the components differing in other characteristics. E.g., the combined chromatographic technique can be employed for the analysis of block copolymers because the separation can be tuned and focused on structural features of one of blocks only.

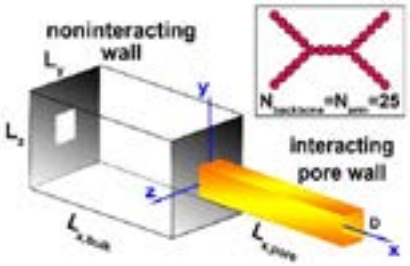

Figure1: *Schematic illustration of the simulation box. Insert shows one of studied branched structures.*

Biography

Karel Procházka is a Professor and Head of "Soft Matter" research group (earlier "Laboratory of Specialty Polymers") at the Department of Physical and Macromolecular Chemistry of the Charles University in Prague. He is a member of the American Chemical Society, Czech Chemical Society and the Czech Learned Society. He has been studying the Conformational and Self-assembling Behavior of Block Copolymers and Polyelectrolytes by a number of experimental techniques, such as Light Scattering, Small Angle Neutron and X-Ray Scattering, Spectroscopy, Size-Exclusion Chromatography, Ultracentrifugation, Colorimetry and Microscopy in combination with Computer Modeling (Monte Carlo simulations, Molecular Dynamics and Self-Consistent Field Calculations). He published more than 150 original publications in recognized impacted journals. His publications are highly cited by other authors (more than 2500 citations by other authors), and contributed to the broadening of the knowledge on the Stimuli-Responsive Self-Assembling Polymer Systems.

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