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1 Using Molecular Simulations to Probe Pore Structures
2 and Polymer Partitioning in Size Exclusion
3 Chromatography

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11 **Abstract**

12 Molecular simulations have been extensively utilized to understand and predict
13 the polymer partitioning in size-exclusion chromatography (SEC). However, ide-
14 alized pore models (e.g., cylindrical, spherical, and slit pores) were often used to
15 represent the porous media in an SEC column, which leads to significant devia-
16 tions in describing the geometry and the size of the pores. In this work, several
17 complex pore models were derived from body-centered cubic, random, and gel
18 packing of monodisperse spherical sol particles using simulation methodology.
19 The mechanical stabilities of these structures were determined based on particle
20 coordination numbers. Pore size distributions of these porous structures were
21 compared to a commercially available, wide-pore superficially porous particle.
22 Then, Gibbs ensemble Monte Carlo simulations were performed to compute the
23 pore-to-bulk partitioning coefficient K_{SEC} of a polymer chain with complex pore
24 models. The effects of particle size, packing structure, and porosity on K_{SEC}
25 were explored. In addition, structural analysis provides insight into the con-
26 formation of polymers in the pores and its effect on the partitioning behavior.
27 This study promotes the understanding of pore structures in SEC columns and
28 enables more accurate predictions of K_{SEC} with less ambiguity in pore geometry.

29
30 **Highlights**

- 31 • Monte Carlo simulation methods were employed to generate various pore
32 structures.
- 33 • Compared size distribution of pore structures with that of an experimental
34 column.
- 35 • Calculated the partition coefficient of polymers for the generated pore
36 structures.
- 37 • Polymers with and without excluded volumes were used in the simulations.

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