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What is the critical condition for equilibrium partitioning of SAW chains into pores? WENHUA JIANG, SCOTT ORELLI, YONGMEI WANG, Department of Chemistry, The University of Memphis, Memphis, TN 38152 — The critical condition of polymer chains partitioning into pores refers to the point at which the entropy loss is compensated by enthalpy gain. This is thought to occur at the critical adsorption point (CAP) of the chain above a solid planar surface and at this point the equilibrium partition coefficient K =1 and is independent of chain length. We investigated this issue by examining the equilibrium partitioning of a SAW chain into a square channel, which mimics the microporous media better than a slit. The partition coefficient of a SAW chain at CAP determined earlier was found to vary dramatically with the chain length in a narrow square channel. As a result, the critical condition point relevant to the experiments can not be defined as the critical adsorption point. Instead, the critical condition point can be identified clearly from the plot of root-mean square deviation in $\ln K$ for a given range of chain length against the surface/bead interaction energy $\varepsilon_{w.}$The critical condition point thus found, ε_w^{cc}, was more attractive than the critical adsorption point. The narrower the channel is, the more attractive the surface interaction would be at the critical condition point.

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