Multi-Scale modeling approach about the behavior of polymers in Supercritical fluilds

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In recent years, molecular simulation methods such as molecular mechanics(MM), molecular dynamics(MD), and Monte Carlo simulation(MC) have been applied to several polymer systems. The method becomes a powerful tool in polymer science, complementing both analytical theory and experiment, but at the same time it has a serious limitation in the space and time scale it can cover.
The equation-of-state (EOS) theory for polymers has been developed as a useful tool to give information on equation-of-state properties. The theory, however, requires tedious experiments to determine the characteristic parameters when dealing with a new polymer.
Thus, it will be helpful if molecular simulation methods can provide the characteristic parameters without experimental efforts. As an exploratory work(multi-scale modeling approach) to combine the EOS theory and the molecular simulation methods, the characteristic parameters were first determined by molecular simulations, and then the behavior of polymers in supercritical fluids was predicted and compared with experimental results.