MONTE CARLO SIMULATION OF METHANOL DIFFUSION IN SUPERCRITICAL FLUIDS

Yu-Xiang Jia Xiang-Yun Guo Bing Zhong*

State Key Laboratory of Coal Conversion, Institute of coal Chemistry, CAS, Taiyuan, 030001, China

zhongb@sxicc.ac.cn

Supercritical fluids (SCFs) have been widely applied in many fields during the last decades. The properties of low viscosity, high diffusivity and adjustable solvency have resulted in numerous applications, e.g., media of chemical reactions, adsorption/separation process and extraction process. For a given process, however not all supercritical fluids produce desirable results. Recently we studied the methanol synthesis in supercritical fluids n-pentane, n-hexane, n-heptane and acetone. It was found that the conversion and selectivity of methanol was remarkably improved only in supercritical hexane. To understand the process from molecular level, the self-diffusion constants of methanol in different supercritical fluids were studied by the Monte Carlo method.

Through modeling the diffusion of methanol in SCFs, the mean square displacement (MSD) of methanol molecule in different time can be obtained, as shown in Fig.1. Based on Einstein's equation, the diffusion constant D can be estimated from Fig.1 and summarized in Table 1. From the table, it is found that the diffusion rate of the methanol in n-hexane is much higher than those in other solvents.

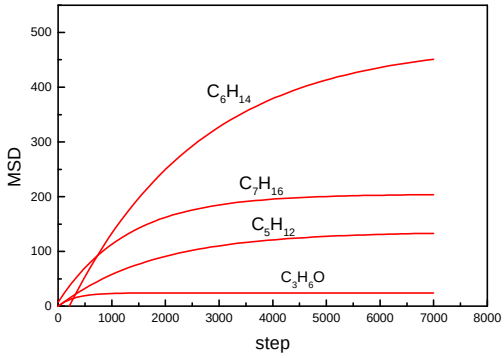

Fig.1. MSD at the critical density of n-pentane, n-hexane, n-hetpane and acetone.

Table 1 Diffusion coefficient D for 800ps

	n-C_5H_{12}	n-C_6H_{14}	n-C_7H_{16}	C_3H_6O
Density (g cm^{-3})	0.234	0.223	0.233	0.278
D (10^{-8} m^2 s)	0.29	1.22	0.31	0.032

The calculated results are consistent with our experiments, which indicated that n-hexane was the best supercritical medium among other SCF media for the reaction of methanol synthesis. From the calculation, it is concluded that the supercritical hexane enhances the desorption of methanol molecules from the catalyst surface and then promotes the conversion of the reaction due to the high diffusivity of methanol in the medium.