中国化学工程学报 2001 9 (2): 196-199 ISSN: 1004-616x CN: 44-1063/R

RESEARCH NOTES

苯在超临界水中的分子动力学研究

周健, 汪文川, 仲崇立

College of Chemical Engineering, Beijing University of Chemical Technology, Beijing 100029, China

收稿日期 修回日期 网络版发布日期 接受日期

摘要 Microscopic structure and diffusion properties of benzene in ambient water (298 K, 0.1 MPa) and super critical water (673－773 K, 25－35 MPa) are investigated by molecular dynamics simulation with site-site models. It is found that at the ambient condition, the water molecules surrounding a benzene molecule form a hydrogen bond network. The hydrogen bond interaction between supercritical water molecules decreases dramatically under supercritical conditions. The diffusion coefficients of both the solute molecule and solvent molecule at supercritical conditions increase by 30－180 times than those at the ambient condition. With the temperature approaching the critical temperature, the change of diffusion coefficient with pressure becomes pronounced.

关键词 supercritical water benzene diffusion coefficients molecular dynamics molecular simulation

分类号

DOI:

Molecular Dynamics Investigation of Benzene in Supercritical Water

ZHOU Jian, WANG Wenchuan, ZHONG Chongli

College of Chemical Engineering, Beijing University of Chemical Technology, Beijing 100029,
China

Received Revised Online Accepted

Abstract Microscopic structure and diffusion properties of benzene in ambient water (298 K, 0.1 MPa) and super critical water (673－773 K, 25－35 MPa) are investigated by molecular dynamics simulation with site-site models. It is found that at the ambient condition, the water molecules surrounding a benzene molecule form a hydrogen bond network. The hydrogen bond interaction between supercritical water molecules decreases dramatically under supercritical conditions. The diffusion coefficients of both the solute molecule and solvent molecule at supercritical conditions increase by 30－180 times than those at the ambient condition. With the temperature approaching the critical temperature, the change of diffusion coefficient with pressure becomes pronounced.

Key words supercritical water; benzene; diffusion coefficients; molecular dynamics; molecular simulation

通讯作者:
周健
作者个人主页: 周健; 汪文川; 仲崇立