Diffusion of Oxygen in Supercritical Water: A Molecular Dynamics Simulation

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Supercritical water attracts a lot of academic and industrial interest because of its unique properties. The diffusion process of oxygen in supercritical water is of great importance in SCWO and corrosion prevention in supercritical power generation. In this paper, molecular dynamics simulations are performed to determine the diffusion coefficients of oxygen molecular in a series of states of supercritical water, covering a wide density range form $0.1 g/cm^3$ to $1 g/cm^3$ and temperature range from 650 K to 950 K. The water molecules in the simulations are described by the SPC model, and the Lennard-Jones potential is employed to calculate the interactions between the oxygen molecules. The Lorentz-Berthelot combining rule is applied to compute the interactions between the water and the oxygen molecules. Simulations are performed under NVT ensemble, applying the Nose-Hoover thermostat. The Ewald sum is used to calculate the long-rang correction for Coulomb potential. Each MD simulation runs over an average period of 300ps after a typical equilibrium procedure of about 150ps, with a time step of 1fs. The diffusion coefficients are calculated from the velocity autocorrelation function and the mean square displacement, which give almost the same results. The temperature and density dependences of the diffusion coefficient are obtained. The results are also analyzed and compared with the experiment data and other MD simulations in literature.