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Molecular dynamics simulation for vapor-liquid coexistence of water in nanocylinder TOSHIKI MIMA, IKUYA KINEFUCHI, YUTA YOSHIMOTO, NOBUYA MIYOSHI, Department of mechanical engineering, University of Tokyo, Bunkyo-ku, Japan, AKINORI FUKUSHIMA, TAKASHI TOKUMASU, Institute of fluid science, Tohoku University, Sendai-shi, Miyagi, Japan, SHU TAKAGI, YOICHIRO MATSUMOTO, Department of mechanical engineering, University of Tokyo, Bunkyo-ku, Japan — Molecular dynamics simulation was conducted in order to investigate the vapor-liquid coexistence of the water molecules in nanopore. In this research, the Lennard-Jones energy parameter between a water molecule and an atom of nanopore was optimized so as to model the contact angle between a water droplet and the carbon material in the fuel cell. The TIP4P/2005 as the model of a water molecule was used; this model produces well the vapor-liquid coexistence line. All of the systems were equilibrated by Nosé-Hoover thermostat. The electrostatic interaction between water molecules was calculated through smooth particle mesh Ewald method. First, we equilibrated a water plug in the single-wall atomistic nanocylinder as a model of nanopore in the fuel cell with radius 1.3nm. Water molecules burst from an interface of the water plug in equilibration. Then, the equilibrium densities both in dense and dilute region ware sampled over 1 ns. The vapor-liquid coexistence line, density profile, free energy profile will be presented in the session.

Toshiki Mima
Dept of mechanical engineering, University of Tokyo, Bunkyo-ku, Japan

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