Molecular dynamics simulation for self-diffusion coefficients of ginger bioactive compounds in subcritical water with and without ethanol

ABSTRACT

Molecular dynamics simulation was used to calculate the self-diffusion coefficients of ginger bioactive compounds (6-gingerol and 6-shogaol) in subcritical water with the presence of ethanol as an entrainer (0–10 mol%) at temperatures from 373.15 to 453.15 K. The all-atom optimised-potentials (OPLS/AA) were employed for the ginger bioactive compounds and ethanol. The extended simple point charge (SPC/E) model was adopted for water molecules. The self-diffusion coefficients increase from 1.00×10^{-9} to 2.70×10^{-9} m^2/s with increasing temperature from 353.15 to 453.15 K. The self-diffusion coefficients also increase from 1.71×10^{-9} to 3.00×10^{-9} m^2/s with increasing percentage of ethanol from 0 to 10 mol% at 413.15 K. The radial distribution functions between the ginger bioactive compounds and subcritical water (solvent) illustrate a weak interaction between the ginger bioactive compounds and solvent. The interaction increases with addition of ethanol as entrainer.

Keyword: Extraction process; Subcritical water; Self-diffusion coefficient; Ginger bioactive compound; Entrainer; Ethanol