ABSTRACT

Chronic Kidney Disease (CKD) is a non-communicable disease characterized by the accumulation of urea in the body, thus requiring hemodialysis therapy using a semipermeable membrane. Chitosan modification into carboxymethyl chitosan (CMCs) has been proposed to enhance membrane–urea interactions through the introduction of carboxymethyl groups. The position of the carboxymethyl substituent in CMCs may influence the effectiveness of urea diffusion. This study aims to investigate the effect of different substitution positions on the interaction energy and energy gap of CMCs with urea using quantum mechanics, as well as to determine the solvation and diffusion coefficient of urea using classical mechanics. Quantum mechanical calculations were performed on O-CMCs, N-CMCs, N,O-CMCs, and N,N-CMCs employing the DFT method with the B3LYP/6-31++G** basis set and D3 correction. Molecular dynamics simulations were conducted using OPLS-AA force field parameterization with the SPC/E water model, 5-mer CMCs, and 10 or 50 urea molecules. The simulation stages included minimization, equilibration (NVE, NVT, NPT), and production (NVE) for 5 ns at 310.15 K. The results revealed that N,N-CMCs exhibited a moderate interaction energy of –69.96 kJ/mol and the lowest energy gap before (4.925 eV) and after interaction (5.192 eV), indicating stable interactions while facilitating urea release. In classical simulations, N,N-CMCs provided optimal urea solvation and achieved the highest diffusion coefficient of 4.516×10^{-5} cm²/s. Therefore, N,N-CMCs represent the most promising functional group position for application as a hemodialysis membrane.

Keywords : hemodialysis, membrane, CMCs, urea, diffusion