**Influence of surfactant for improving dewatering of brown coal: A comparative experimental and MD simulation study**

**Objective**

In this study, a molecular level description of the interactions of the lignite/surfactant/water system is provided by MD simulation.

**Methodology**

The COMPASS force field was employed in MD simulations. 80 optimized lignite molecules were put into a periodic box. In the case of a constant pressure-temperature ensemble with the Berendsen thermostat and barostat, the system was equilibrated. The temperature of the system was maintained at 298 K and the pressure was set to 0.1 MPa. A time step of 1.0 fs was employed to integrate the motion equations. The Ewald Summation method and a van der Waals interaction cutoff of 12.5 Å were used to account for long-range electrostatic interactions. After an equilibration time of 500 ps in the NPT ensemble, the brown coal model was constructed. The coal-water-TX system, which included 80 brown coal macromolecules, 5000 water molecules, and 3 TX-100 molecules, was packed into a rectangular simulation cell with dimensions of 44.74 × 44.74 × 150 Å3 (X × Y × Z). The simple point charge (SPC) water model was adopted. The simulation was performed in the NVT ensemble level at 298 K using a Nose thermostat with time step of 1.0 fs. A van der Waals interaction cutoff of 12.5 Å and the Ewald summation method, with an accuracy of 10-3 kcal/mol, were employed to account for long-range electrostatic interactions. The bottom of the lignite model was frozen during the simulation to reduce computational cost. The simulation was run for 1 ns and the final results were obtained from simulations of 500 ps.

**Findings**

The density distributions of lignite, TX-100 and water molecules along the Z-axis showed that TX-100 molecules adsorbed at the water-coal interface. It means that TX- 100 molecules repelled water molecules near lignite surface. The aggregated structure of adsorbed TX-100 molecules shows that the ethoxylate groups are closer to the coal surface than that of octylphenol groups. The mobility of water molecules was enhanced in presence of TX-100 according to the results of mean square displacement (MSD) and diffusion coefficient.