**Molecular dynamics simulations of interaction between sub-bituminous coal and water**

**Objective**

In this study the interactions between sub-bituminous coal and water were analyzed by using molecular dynamics simulations.

**Note:** Because of complex composition and structure, the graphite surface modified by hydroxyl, carboxyl and carbonyl groups was used to represent the surface model of sub-bituminous coal according to XPS results.

**Methodology**

Molecular dynamics simulations were conducted using the Materials Studio 8.0 package. The COMPASS force field was applied for all simulations. The graphite is composed of four graphene sheets separated by 3.4 Å from each other. The hydroxyl, carboxyl and carbonyl groups were randomly grafted to the carbon atoms on the first graphene basal plane. The water molecules were simulated using the simple point charge/extended (SPC/E) model. The simulation box was built by placing one slab of the solid substrates at the base and another, specularly symmetric, at a distance *H* = 70 Å along the *z* axis. The solid substrate is aligned parallel to the *x* and *y* plane, and the *x* and *y* dimensions are 25.6 and 29.5 Å, respectively. The number of water molecules was 1000, which were placed on the solid substrate. Periodic boundary conditions were applied along the *x*, *y* and *z* axes. All simulations were performed at NVT ensemble at 298 K using a Nose thermostat, and the time step is set to 1.0 fs. A van der Waals interaction cut-off of 12.5 Å was employed, and the Ewald summation method with an accuracy of 10-3 kcal/mol was used to account for the long-range electrostatic interactions. The final results are calculated based on the production of 500-ps simulation after the equilibration period.

**Findings**

The oxygen and hydrogen atomic density data show the formation of two hydration layers. The results of radial distribution functions, mean square displacement and local self-diffusion coefficient for water molecules related to three oxygen moieties confirmed that the water molecules prefer to absorb with carboxylic groups, and adsorption of water molecules at the hydroxy and carbonyl is similar.