Study on the Influence of Surfactants on the Wettability of Coal Dust Based on Molecular Dynamics Simulation

Y Zhang1,2, L Yuan3 and T Ren4

Note: Presenting author’s name should be underlined.

1. PHD Student, Anhui University of Science and Technology, Huainan China 232001. Email: ahzhangyi11@163.com

2. Joint PHD Student, University of Wollongong, New South Wales 2500. Email: yz062@uowmail.edu.au

3. President, Anhui University of Science and Technology, Huainan China 232001. Email: yuanl\_1960@sina.com

4. Professor, University of Wollongong, New South Wales 2500. Email: tren@uow.edu.au

Keywords: Coal dust, Molecular dynamics simulation, Wettability

# ABSTRACT

In coal mine dust control, techniques such as spray dust suppression and coal seam water injection are commonly employed, with dust removal efficiency serving as a key determinant of control effectiveness. However, the detailed mechanism by which surfactant molecules interact with water molecules to wet coal powder in solution has been less frequently explored. Advances in computational technologies have enabled the application of mature molecular dynamics (MD) simulation techniques, which have proven to be powerful tools for elucidating intermolecular interactions at the microscopic level. In the field of coal mine dust prevention and control, MD simulations are widely utilized to investigate the wetting effects of surfactants on coal surfaces. These studies often focus on enhancing wettability, and the changes in contact angles between coal particles and liquid droplets. Such research provides deeper insights into the relationship between coal structure and wettability modifications. Overall, molecular dynamics simulations offer a precise microscopic perspective for studying coal wettability. When combined with experimental validation, these simulations help optimize dust removal technologies and surface modification processes. Additionally, recent studies have explored the influence of surfactant-modified nanofluids with drag-reducing properties on coal wettability, revealing potential molecular-level mechanisms through an integrated approach of experimental and computational analysis. This study further explored the effect of surfactant modified nanofluids with drag reducing properties on coal wettability and the potential mechanisms at the molecular level through a combination of experiments and simulations. Molecular simulations were conducted with molecular simulation software to construct H2O/Coal, H2O/AOS/Coal, and H2O/AOS-modified SiO2/Coal systems. These simulations were intended to explore the synergistic effect between SiO2 nanoparticles and surfactants, as well as changes in the adsorption configuration, relative concentration distribution, and MSD of water molecules within their composite systems. The research results of this study will provide valuable information for the application of nanofluids in coal mine dust prevention and control.