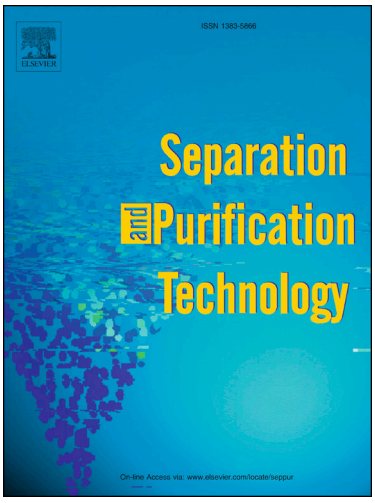

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Influence of surfactant for improving dewatering of brown coal: A comparative experimental and MD simulation study

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Abstract Experimental method and molecular dynamics (MD) simulations were used to investigate the filtration dewatering process of brown coal in the presence of the surfactant TRITON X-100 (TX-100). A significant reduction in filter cake moisture content was observed upon addition of TX-100 in the dewatering experiments. It was observed that a narrow TX-100 concentration range of below the critical micelle concentration (CMC) was best for dewatering. The enhancement in filtration dewatering characteristics could be attributed to the wetting characteristic changes of the brown coal surface caused by surfactant adsorption, as indicated by measurement of contact angles. Monolayer adsorption of TX-100 at the lignite surface was investigated by MD simulations. The TX-100 molecules repelled water molecules near the coal surface and adsorbed at the water-lignite interface with the ethoxylate closer to the coal surface than the octylphenol. The mobility of water molecules was enhanced in presence of TX-100 according to the results of mean square displacement (MSD) and diffusion coefficient. It was inferred that adsorption of TX-100 resulted in a more hydrophobic brown coal surface, in agreement with the dewatering and contact angle experiments.

Keywords lignite; dewatering; surfactant; molecular dynamics; contact angle

1. Introduction

Brown coal reserves are estimated at 1025 billion tons worldwide, accounting for nearly 40% of all coal reserves [1]. However, its high moisture content hinders the efficient use of brown coal. The high moisture content increases the costs of transportation and storage of the coal. Besides, the high moisture affects the thermal efficiency of power generation [2, 3]. When brown coal is

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