Monte Carlo Simulation of Interlayer Molecular Structure in Swelling Clay Minerals. 1. Methodology

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Abstract: Monte Carlo (MC) simulations of molecular structure in the interlayers of 2:1 Na-saturated clay minerals were performed to address several important simulation methodological issues. Investigation was focused on monolayer hydrates of the clay minerals because these systems provide a severe test of the quality and sensitivity of MC interlayer simulations. Comparisons were made between two leading models of the water-water interaction in condensed phases, and the sensitivity of the simulations to the size or shape of the periodically-repeated simulation cell was determined. The results indicated that model potential functions permitting significant deviations from the molecular environment in bulk liquid water are superior to those calibrated to mimic the bulk water structure closely. Increasing the simulation cell size or altering its shape from a rectangular 21.12 Å x 18.28 Å 6.54 Å cell (about eight clay mineral unit cells) had no significant effect on the calculated interlayer properties.

Key Words: Clay-water systems • Monte Carlo simulation • Swelling clays

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