Monte Carlo Computer Simulation on Phase Equilibria of Geological Fluids

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A new method (Gibbs Ensemble computer simulation) has been used to simulate the phase equilibria of the natural fluid system CO_2–CH_4–N_2 over a wide temperature-pressure-composition range. The phase behavior (the equilibrium composition and density) can be observed from the simulation with accuracy close to experiments. It is remarkable because the simulation are solely based on two molecular interaction parameters. Comparison with the most popular equations of state (EOS) for the above system indicates that the simulation in general gives better predictions. The simulated data can be used in the study of geological fluid inclusions and in the recovery of methane from CO_2-containing natural gas by cryogenic processing. This method can be used to study phase behavior of other natural fluid systems under experimentally difficult conditions.