1135-86-3125 **Jose Navarro Nunez*** (jnavarronunez@sdsu.edu), San Diego State University, 5500 Campanile Drive, San Diego, CA 92182-1326, and **Christopher Paolini** (paolini@engineering.sdsu.edu) and **Jose Castillo** (jcastillo@mail.sdsu.edu). *Parallelized Chemical Equilibrium Solver for Geologic CO2 Sequestration.*

Thermochemical processes occurring during geologic CO2 sequestration have varying characteristic time scales. While the mineral trapping of CO2 occurs over many years, there are chemical reactions involved that reach an equilibrium state much sooner. For these reactions, it is safe to ignore the chemical kinetics involved and directly compute the equilibrium composition. We present a chemical equilibrium solver that computes the chemical species composition, pH, alkalinity, and redox potential of a NaCl-H2O-CO2 system. The equilibrium model is based on the minimization of the system Gibbs free energy through the method of augmented Lagrange multipliers. In order to obtain accurate results at the extreme thermophysical conditions encountered in the subsurface, the Pitzer model is used to calculate chemical species activity. The equilibrium solver is parallelized, using OpenMP and MPI, to handle a large number of chemical species and virial terms for the Pitzer equations. The methods implemented are high-level OpenMP and vectorization on Intel's Xeon Phi Knights Landing architecture. (Received September 26, 2017)