Improved Thermodynamic Model for Aqueous NaCl Solutions from 350 to 400 °C

B. Liu[S], J.L. Oscarson[C] and C.J. Peterson
Department of Chemical Engineering, Brigham Young University, Provo, UT, U.S.A.
oscarj@et.byu.edu

R.M. Izatt
Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, U.S.A.

A model, based on Helmholtz energy, that can be used to describe thermodynamics of NaCl solutions in the water near-critical region has been developed and tested as a function of temperature (350 to 400 °C), pressure (18 to 41 MPa), and solute concentration (0 to 5 molal) using literature densities, apparent NaCl(aq) molar volumes, heats of dilution, and apparent isobaric molar heat capacities. Densities, heats of dilution, apparent molar isobaric heat capacities, and apparent NaCl(aq) molar volumes calculated using the model are in agreement with literature values over the conditions studied. Calculated apparent molar isobaric heat capacities agree with literature data up to 450 °C even though the data used in model regression were valid only at temperatures from 350 to 400 °C. Since calculation of apparent molar isobaric heat capacities involves the second temperature derivative of Helmholtz energy, extrapolation to temperatures > 400 °C should give reasonable results.