Predicting Aqueous Electrolyte Solution Density Between (273 and 373) K and up to 100 MPa

Darren Rowland [C, S] and Peter M. May
Department of Chemistry, Murdoch University, Murdoch, Western Australia, Australia
d.rowland@murdoch.edu.au

Densities / volumes are among the most commonly reported physicochemical properties of aqueous electrolyte solutions in the chemical literature. Apart from their intrinsic value, volumetric information is useful for calculating changes to electrolyte activity and solubility when systems are subjected to high pressure, such as occurs in seawater and deep geological brines. While the major sea salts have been the focus of many experimental studies at high pressure and over a range of temperature, unfortunately, reliable density information for most other salts is lacking for conditions away from ambient. Thus, there is a need for well-founded approaches to estimating the volumetric properties of aqueous electrolyte solutions and their mixtures as functions of pressure and temperature. This work describes an investigation into methods of obtaining solution densities in both the temperature and pressure domain based on (i) having limited numbers of experimental data available at 298 K and 0.1 MPa, and (ii) empirical trends that have been observed for the best-characterized electrolyte solutions in the pressure and temperature range of interest. The predictions are validated against authoritative volumetric data for binary and multicomponent electrolyte solutions at pressures up to 100 MPa and temperatures from (273 to 373) K.