A New Type of Aqueous Phase Diagram

Klaus Hack, GTT-Technologies

Phase diagram sections of aqueous systems are calculated thermodynamically employing data from large evaluated databases. Axes and constants can be temperature, mass or molar ratios, and/or chemical potentials for systems of any number of components and with non-ideal solutions. Iso-*Eh* and Iso-pH lines are calculated and plotted. The equilibrium amounts, and compositions of all phases can be readily displayed at any point on a diagram. The diagrams, once calculated, can be re-plotted in *Eh*-pH coordinates if appropriate x- any y-axes have been