

## **Aqueous solution database and modelling using the Pitzer formalism and ChemApp/ ChemSheet**

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Together with high temperature systems, aqueous solutions are among the most important application areas of multicomponent, multiphase thermodynamic modelling. Within area of aqueous solution thermodynamics, the Pitzer model is likely the most commonly used as it offers application range from dilute to fairly concentrated solutions and a large number of available published parameters.

The presentation covers general common features of aqueous solution models and activity coefficients when applying the Pitzer model together with some of the available data sources as well database development work done at VTT targeting at chloride, carbonate and sulphate containing process solutions with Na, K, Ca, Mg, Al, Fe, Cu, Mn metal cations within the temperature range of 25-100 °C.

Also discussed are advanced features such as pH target calculation within ChemApp calculations and handling of supersaturated solutions.