Further Development of THEREDA database in SysCAD for aqueous/brine applications

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SysCAD is a process simulation software package featuring a Thermodynamic Calculation Engine (TCE) interface which communicates with ChemApp. The combination of SysCAD functionality and ChemApp thermodynamic calculations via the TCE interface makes a powerful analysis tool for a host of chemical processes. In this work the THEREDA database (developed by GRS, HZDR, KIT, TUBAF, and CSD Engineers) is used by ChemApp within a SysCAD process simulation to predict the performance of a muriate to sulphate of potash conversion process (as proposed by Fabrik et al, 2017). Model predictions are used to calculate the optimal sodium sulphate reagent dosage as a function of process operating temperature. It is found that, as temperature increases, the potassium sulphate yield is reduced.