Screening of Electrolyte Solutions as Phase Change Materials using COSMO-SAC and Numerical Optimization

Erik Mickoleit[1, S, C], Tommy Lorenz[1], Marcel Felix Schneegans[1], Sebastian Pinnau[1] and Cornelia Breitkopf[1]

[1]*Technische Universität Dresden, Dresden, Germany*
erik.mickoleit@tu-dresden.de

Due to climate change, an increased demand for cooling while trying to reduce overall greenhouse gas emissions seems to be a contradiction. Phase change materials (PCMs) as latent heat storage materials have been of scientific and commercial interest for years. PCMs can help provide environmentally friendly cooling in buildings by acting as a heat sink during the day by melting the PCM and regenerating at night by crystallizing. For optimal use, such PCMs must have a melting temperature adapted to the desired application conditions. Salt hydrates can be a suitable candidate PCM with a high specific heat storage capacity. The melting temperature and thus the application temperature can be adjusted by mixing different salts in aqueous solutions. To drastically reduce the experimental effort, a theoretical screening of suitable salt hydrates was performed. Excess Gibbs energy data obtained by the Conductor-like Screening Model – Segment Activity Coefficient (COSMO-SAC) for electrolyte solutions [1] were converted to Redlich-Kister-Muggianu parameters [2,3] and used in the FactSage software tool to calculate phase diagrams [4]. The standard enthalpy and entropy at infinite dilution for aqueous salt solutions were adjusted using FactSage's CalPhaD (Calculation of Phase Diagrams) optimizer for later application to aqueous salt mixtures. An extensive database of salt hydrate mixtures based on the system Na^+, K^+, Ca^{2+}, Mg^{2+} // Cl^-, NO_3^-, SO_4^{2-}, CO_3^{2-} // H_2O was built to screen for suitable PCMs.

References

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