Kurzfassung: Ermittlung von Stoffpaaren für Absorptionswärmepumpen mit Hilfe von prädiktiven Modellen / Determination of working pairs for absorption heat pumps using predictive models

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Absorption chillers and heat pumps have been analyzed as an alternative to compression refrigeration machines to provide heat and cold. This work examines the substance class of ionic liquids in the working pair of refrigerant and absorption media for absorption chillers (AWP Type I) and heat transformers (AWP Type II) to substitute water / lithium bromide (LiBr), which suffers from drawbacks like low efficiency, corrosiveness, crystallization and large system size. A method is developed to identify competitive working pairs to water / LiBr with high performance (high COP, low solution circulation ratio). A fully predictive concept is presented based on process simulation and COSMO-RS derived activity coefficients.

Comparing literature data to data derived using COSMO-RS, sequencing is predicted well, though the difference of the simulated maximum COP was up to 6 % for AWP Type I and 7 % for AWP Type II. Whereas, the standard deviation for the COP was 0.04 for AWP Type I and 0.03 for AWP Type II. Sensitivity analysis showed that substance properties impact the COP significantly in comparison to the apparatus' properties (like heat exchanger efficiency). As the refrigerant properties enthalpy of vaporization and heat capacity are critical regarding COP, water is the refrigerant of choice for domestic applications. Thus, performance increase must be achieved via the absorption medium, ionic liquid. Selection criteria to reduce the number of potential working pairs were analyzed subsequently. It could be shown that via the decrease of the partial pressure in dependence of the composition the sequencing of working pairs regarding the COP could be estimated. Using the activity coefficients at infinite dilution, it could be shown that classification of working pairs in three classes made it possible to distinguish different solution types with characteristic potential in absorption heat pumps. Further differentiation could be achieved using the information of molecular weight and heat capacity of the ionic liquids. It was found that the impact of the heat capacity was bigger for working pairs with small attractive interactions with the refrigerant, although the impact is small in general.

Three candidates derived from the presented method were compared to the benchmark process water / LiBr. It could be shown that working pairs of similar performance were detected. For AWP Type I water / LiBr ($COP_{max} = 0,83$) could be substituted by water / [N1111][C1SO3] ($COP_{max} = 0,79$), water / [N1111][Nitrat] ($COP_{max} = 0,79$) or water / [N1132OH][C1SO4] ($COP_{max} = 0,87$). Water / [N1111][2C1PO2] ($COP_{max} = 0,51$), water / [N1111][HCO3] ($COP_{max} = 0,50$) and water / [N1111][Nitrat] ($COP_{max} = 0,49$) could compete with water / LiBr ($COP_{max} = 0,49$) in AWP Type II.