Determination of solution/solute interface parameters from measured deliquescence/efflorescence humidities

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For investigation of growth/shrinking of a hygroscopic nanoparticle during hydration/dehydration in a water vapour atmosphere we have used a thermodynamic approach of Shchekin, Shabaev, and Rusanov (2008). It employs the concept of disjoining pressure of thin films and allows the prediction of the humidity growth factor (HGF) of both (i) a homogeneous solution droplet with completely dissolved residual core, and (ii) a heterogeneous solution droplet with partially dissolved residual core as a function of the ambient relative humidity. For application to a nanometric NaCl particle we have extended the original approach by (i) consideration of the nonideality of the solution and by (ii) derivation of an additional equation for the estimation of the efflorescence properties of a homogeneous solution droplet. It will be demonstrated how the solution/solute interface energy and the correlation length of a thin solution film can be determined from a combination of experimentally determinable efflorescence and deliquescence humidities (ERH, DRH) with the present calculus.

For a NaCl particle with dry particle radius of 5 nm the solution/solute interface energy was estimated to be 0.088 Jm^{-2}, which is in close agreement with some previous values reported in the literature but which strongly differs from data of some other sources. The film correlation length was estimated to be 1 nm, which is reconcilable with data from previous computer simulations when the measurement uncertainty of the deliquescence humidity is taken into account.

Considering the combination of an extensive calculus, a comprehensive set of thermophysical constraints, and independent measurements of the deliquescence and efflorescence humidities as functions of dry particle radius, the obtained values of the solution/solute interface energy and the correlation length are in close agreement with previous estimations.

In the presentation we will give an overview of the calculus and discuss the calculated HGF on the base of numerical solution of generalised Gibbs-Kelvin-Köhler and Ostwald-Freundlich equations (see Fig. 1) and together with other physicochemical parameters.

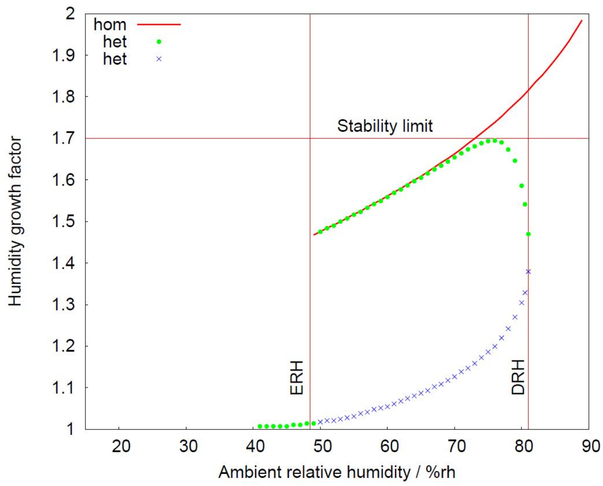

Figure 1. Calculated HGF as function of ambient relative humidity for a NaCl particle with dry particle radius of 5 nm. The red solid line represents the HGF of a homogeneous solutions droplet, the green and blue dotted lines that of a heterogeneous solution droplet.

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