

## Saturation vapour pressures of subcooled liquid oxodicarboxylic acids

I. Crljenica<sup>1,6</sup>, T. Yli-Juuti<sup>2</sup>, A.A. Zardini<sup>3,4</sup>, J. Julin<sup>1,6</sup>, M. Bilde<sup>5</sup>, I. Riipinen<sup>1,6</sup>

<sup>1</sup>Department of Applied Environmental Science (ITM), Stockholm University, 10691 Stockholm, Sweden

<sup>2</sup>Department of Physics, University of Helsinki, P.O. Box 64, 00014 Helsinki, Finland

<sup>3</sup>Department of Chemistry, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark

<sup>4</sup>Institute for Energy and Transport, Sustainable Transport Unit, European Commission Joint Research Centre, 21027 Ispra, Italy

<sup>5</sup>Department of Chemistry, Aarhus University, Langelandsgade 140, 8000 Aarhus, Denmark

<sup>6</sup>Bert Bolin Centre for Climate Research, Stockholm University, 10691 Stockholm, Sweden

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Presenting author email: ivica.crljenica@itm.su.se

Atmospheric aerosols contain a significant mass fraction of organic particles which are composed of a large number of compounds with varying and poorly known physical properties (Jimenez *et al.*, 2009). In this study we estimate the saturation vapour pressure of low volatility organic compounds present in the atmosphere by interpreting the evaporation experiments of oxodicarboxylic acid aqueous solution droplets at ambient temperature. The modelling of evaporation is done with a two-compartment binary mass transport model including group contribution methods parametrizations for the physical properties of the organic acids.

The experimental data (particle diameter vs. time) were obtained from a TDMA system including a controlled-humidity isothermal laminar flow reactor (Bilde *et al.*, 2003). The evaporation was modelled with a two-compartment (the liquid bulk of the aerosol particle and the gaseous surroundings) binary mass transport model with fixed relative humidity and temperature, and dynamic activity coefficients (Riipinen *et al.*, 2006). The accommodation coefficients were set to unity. A dilution parameter for oxodicarboxylic acid had to be introduced into the model to account for the uncertainty in the gas phase concentrations of the evaporating compounds. The physical properties of pure liquid organic acids used in the model were estimated through group contribution methods (Poling *et al.*, 2007). Activity coefficients, for organic acid and water, were calculated using the UNIFAC Dortmund method (Jakob *et al.*, 2006). Density of pure liquid organic acids was predicted by the GCVOL-OL-60 method (Ihmels *et al.*, 2003). Surface tension at room temperature was estimated with the GC-MG method (Conte *et al.*, 2008). Diffusion coefficients were calculated using the Fuller *et al.* method (Poling *et al.*, 2007). The physical properties of water were calculated by the appropriate methods (Poling *et al.*, 2007). The physical properties of the binary mixture were calculated as a mass weighted average for density, and as mole weighted average for surface tension. The comparison between the experimental data and the model results, assessed through the method of least squares, gave us the value for the saturation vapour pressure of the organic acid.

Figure 1 shows a typical measurement dataset for 2-oxoglutaric acid together with the best modelled

evaporation curve with the subcooled liquid saturation vapour pressure of  $2.61 \cdot 10^{-5}$  Pa. This value can be compared with  $3.2 \cdot 10^{-5}$  Pa for the measured saturation vapour pressure of solid oxoglutaric acid (Frosch *et al.*, 2010), or with  $80 \cdot 10^{-5}$  Pa for the subcooled liquid glutaric acid determined from measurements by using a model similar to the one we used (Koponen *et al.*, 2007), or  $93 \pm 27 \cdot 10^{-5}$  Pa for the measured saturation vapour pressure of subcooled liquid glutaric acid (Soonsin *et al.*, 2010).

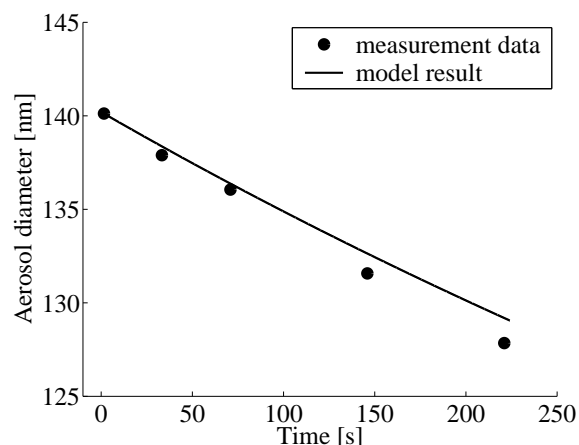


Figure 1. Modelled evaporation curve (line) and the measurements (points) for 2-oxoglutaric acid (relative humidity 40%, long residence time of 222s).

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