

Using tephra layers to provide absolute and relative chronologies for sedimentary archives: An example from the Lake Suigetsu SG06 record from Japan

V.C. SMITH¹, R.A. STAFF¹, D. F. MARK²,
S.P.E. BLOCKLEY³, C. BRONK RAMSEY¹
AND T. NAKAGAWA⁴

¹Research Laboratory for Archaeology and the History of Art, University of Oxford, Oxford OX1 3QY, U.K.
(victoria.smith@rlaha.ox.ac.uk)

²Scottish Universities Environmental Research Centre (SUERC), East Kilbride G75 0QF, U.K.

³Centre for Quaternary Research, Royal Holloway University of London, Egham TW20 0EX, U.K.

⁴Department of Geography, University of Newcastle, Newcastle Upon Tyne NE1 7RU, U.K.

The Lake Suigetsu SG06 sedimentary archive from Honshu Island, central Japan, provides a high-resolution palaeoenvironmental record for the last 150 kyrs. The 73 m-long record contains numerous layers tephra (30 visible and numerous cryptotephra) sourced from explosive volcanism from Japan and South Korea. These marker layers can be used for both relative and absolute chronology.

The glass chemistry of these tephra is typically unique, therefore most of the layers can be correlated to those in other archives and to specific eruptions [1]. Since many of these layers are widespread (>600 km from source) these isochrons allow for the assessment of leads and lags in palaeoclimate across the region.

The tephra can also be dated using ⁴⁰Ar/³⁹Ar methods. These ⁴⁰Ar/³⁹Ar ages are crucial for constraining the pre-50 ka SG06 age model. Correlating these distal SG06 tephra layers to proximal deposits is essential as large crystals are required to obtain precise and ⁴⁰Ar/³⁹Ar ages and these are only abundant in the coarser proximal deposits [2].

Precise radiocarbon dates have been obtained for all the post-50 ka visible SG06 tephra layers [1] using the modelled radiocarbon data and varve chronology [3]. These radiocarbon dates and ⁴⁰Ar/³⁹Ar ages of the eruptions can significantly improve the age models of other archives in which the tephra are found.

[1] Smith *et al.* (2013) *Quaternary Science Reviews* **67**, 121-137. [2] Smith *et al.* (2011) *Quaternary Science Reviews* **30**, 2845-2850. [3] Bronk Ramsey *et al.* (2012) *Science* **338**, 370-374.

Molecular simulation of aqueous electrolyte solutions

WILLIAM R. SMITH^{1,2}*, FILIP MOUČKA³
AND IVO NEZBEDA⁴

¹University of Ontario Institute of Technology, Faculty of Science;

²University of Guelph, Mathematics and Statistics,
(william.smith@uoit.ca *presenting author)

³J.E. Purkinje University, Physics, (fmoucka@seznam.cz)

⁴J.E. Purkinje University, Chemistry, (inezbeda@icpf.cz)

We employ the Osmotic Ensemble Monte Carlo (OEMC) algorithm [1] to predict the solute and water chemical potentials in aqueous electrolyte solutions. OEMC implements a Semi-Grand Canonical Ensemble simulation of the solution phase, which can be viewed as an application of the Reaction Ensemble Monte Carlo algorithm [2] to the case of an inter-phase chemical reaction, including speciation reactions as appropriate.

Focusing on aqueous NaCl at ambient conditions, we present the following:

1. An improved electrolyte force field based on SPC/E water and a simple charged Lennard-Jones sphere model, determined by fitting the concentration dependence of the density and chemical potential, and the solubility.
2. Calculations of the concentration dependence of the water chemical potential and demonstration of thermodynamic consistency with the electrolyte chemical potential using the Gibbs-Duhem equation.
3. Electrolyte chemical potentials at finite concentrations for polarizable force fields for water and the electrolyte, using the Multi-Particle Move Monte Carlo method [3].
4. Calculations predicting the onset of homogeneous nucleation in supersaturated aqueous electrolyte solutions.

[1] F. Moučka, I. Nezbeda, W.R. Smith, *J. Phys. Chem.* **B116**, 5468 (2012); *idem*, *J. Chem. Phys.*, in press (2013). [2] W.R. Smith, B. Tríska, *J. Chem. Phys.* **100**, 3019 (1994) [3] F. Moučka, M. Rouha, and I. Nezbeda, *J. Chem. Phys.* **126**, 224106 (2007).