# A state-of-the-art report within NEA-TDB to assess modeling and experimental approaches in aqueous high ionic-strength solutions

NEA NUCLEAR ENERGY AGENCY

*OECD/NEA Thermochemical Database Project (TDB)*

M. Altmaier[1], D. Costa[2], A. Felmy[3], H. Moog[4], R. Pabalan[5], M. Ragoussi[2], D. T. Reed[6], W. Runde[7], W. Voigt[8]

*1) KIT-INE, 2) OECD NEA, 3) WSU, 4) GRS, 5) NWTRB, 6) LANL-CBFO, 7) LANL, 8) TUBAF*

**Within the scope of the OECD Nuclear Energy Agency (NEA) Thermochemical Database (TDB) Project, the preparation of a State of the Art Report (SOAR) to assess the modeling and experimental approaches used to describe high ionic-strength solutions is being prepared. This state of the art report builds on past NEA-TDB documents [1] and focuses on ionic strengths I > 3 M where the Pitzer formulation [2,3], rather that the SIT approach, is recommended and usually applied. The focus of this SOAR is on the nuclear waste disposal aspects that apply to repository concepts in bedded and domed rock salt formations, although there is also relevance to other geologic disposal concepts where transient high ionic-strength aqueous conditions can exist. A comprehensive high quality and self-consistent Pitzer data set that can describe the aqueous radionuclide/actinide and brine chemistry for all predicted repository conditions is needed to address low-probability brine-inundation scenarios to support the safety case for a nuclear waste repository in rock salt [4].**

**The following institutions and researchers are contributing to the NEA-SOAR:**

- *Altmaier, Marcus: Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal, Karlsruhe, Germany.*
- *Felmy, Andy: Washington State University, Pullman WA, USA.*
- *Moog, Helge: Gesellschaft für Anlagen- und Reaktorsicherheit (GRS), Braunschweig, Germany.*
- *Pabalan, Roberto: U.S. Nuclear Waste Technical Review Board, Arlington VA, USA.*
- *Reed, Don: Los Alamos National Laboratory, 1400 University Drive, Carlsbad NM, 88220, USA.*
- *Runde, Wolfgang: Los Alamos National Laboratory, Los Alamos NM, 87545, USA.*
- *Thakur, Punam: Carlsbad Environmental Monitoring & Research Center, NMSU, Carlsbad NM, USA.*
- *Wolfgang Voigt, TU Bergakademie Freiberg, Saxony, Germany.*
- *Ragoussi, Marilena, Costa, Davide: OECD Nuclear Energy Agency, Issy-les-Moulineaux, Paris, France.*

**A survey of the literature on the experimental parameter determination and modeling of high ionic-strength solutions showed that there are approaching 2000 publications on these topics (see Figure 1). More importantly many of these are relatively recent (since the year 2000) and are not comprehensively integrated into current data sets.**

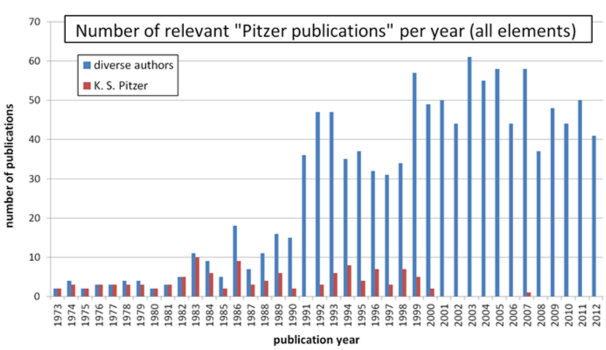


***Figure 1: Publications that center on the experimental measurement of or modeling with Pitzer data since the development of the Pitzer approach in 1973***

**The Pitzer literature that pertains to a nuclear repository in salt was divided into two categories: "Oceanic" for the main components of high ionic-strength brine and "Radionuclide/actinide" for the key radionuclides (and their analogs) that need to be addressed to support the Safety Case. The vast majority of the available literature deals with the brine chemistry associated with "oceanic" systems (~1000 species-specific) and this remains a very active area of research for a number of reasons outside of the nuclear repository application. The distribution of recent publication in this category is given in Figure 2 and shows that there are new activity data being measured as well as new temperature-variable data being reported. All of these data were assessed in the context of current database applications that are largely based on the Harvie-Møller-Weare data base [5].**

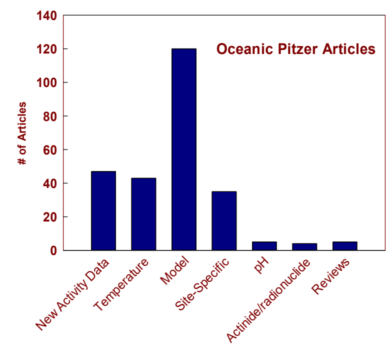


***Figure 2: Distribution of Pitzer articles in the general category of oceanic data studies. Most new activity coefficient data measurements included temperature-variable studies. The vast majority of the papers was the application of the HMW Pitzer model, or optimized versions of this model, to site/system-specific high ionic-strength brines ("Model" designation above).***

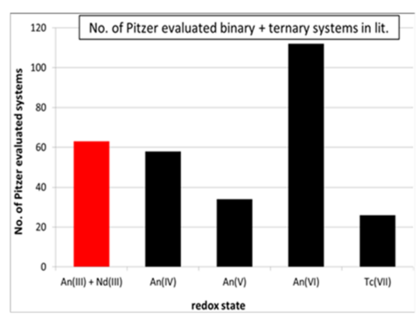


***Figure 3. Number of Pitzer-evaluated binary and ternary system references sorted by oxidation state.***

**For the radionuclide/actinide data set, there are new data reported for all the key oxidation states of the actinides but there are significantly less literature publications (~65) on this key topic (see Figure 3). There is especially a significant lack of temperature-variable data for the radionuclide/actinide data set as well as ternary species and a number of gaps exist in current database applications.**

**The NEA SOAR will provide an overview of existing Pitzer interaction parameters with emphasis on those that are relevant to nuclear waste disposal, will highlight the main achievements and challenges of the application of the Pitzer approach, and conclude with a critical assessment of the key data gaps and modeling limitations/concerns that are identified.**

*References*

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