

Experimental studies on $\text{Th}(\text{OH})_{4(\text{am})}$ solubility in presence of ISA, gluconate or EDTA

E. COLÀS^{1,2*}, M. GRIVÉ¹, I. ROJO^{2,3} AND L. DURO¹

¹Amphos 21, Passeig de Rubí 29-31, 08197 Valldoreix, Spain
(*correspondence: eli.colas@amphos21.com)

²CTM Centre Tecnològic, Av. de les Bases de Manresa 1, 08242 Manresa, Spain

³Chemical Engineering Department, UPC, Av. Diagonal 647 H4, 08028 Barcelona, Spain

The effect of Low Molecular Weight (LMW) organic compounds (as isosaccharinate (ISA), gluconate (GLU) and ethylenediaminetetraacetate (EDTA)) on the mobilisation of radionuclides has been proven to be important. There is a lack of data regarding the stoichiometry and stability of the species formed, especially under alkaline to hyperalkaline conditions [1].

The present work aims at assessing the effect of ISA, GLU and EDTA on the solubility of thorium. Experimental results at pH=12 indicate that ISA, GLU or EDTA concentrations lower than 10^{-3} M have no effect on the solubility of Th. At higher ligand concentrations there is a clear solubility increase with the concentration of organic ligand (see Figure 1). In this case, the formation of 1Th:1L and 1Th:2L complexes (depending on the ligand studied) is suggested.

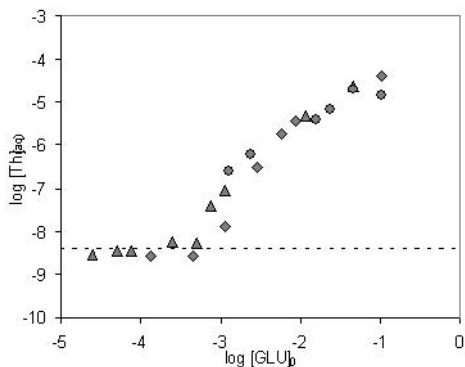


Figure 1: Experimental solubility (symbols) of $\text{Th}(\text{OH})_{4(\text{am})}$ at different Gluconate concentrations (pH=12), and calculated solubility (dotted line) in the absence of organic ligands.

[1] Hummel *et al.* (2005) *Chemical Thermodynamics* **9**, OECD Nuclear Energy Agency.

Structure and dynamics of fluids in nanoporous earth and engineered materials determined from neutron scattering and MD simulations

D.R. COLE^{1*}, E. MAMONTOV¹, G. ROTHER¹,
A.A. CHIALVO¹, L. VLCEK² AND P.T. CUMMINGS²

¹Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA
(*correspondence: coledr@ornl.gov)

²Vanderbilt University, Nashville, TN 37235 USA

The behavior of fluids in confined geometries (pores, fractures) typically differs from their bulk behavior in many ways due to the effects of large internal surfaces and geometrical confinement. Phase transitions (i.e., freezing and capillary condensation), sorption and wetting, and dynamical properties, including diffusion and relaxation, may be modified, with the strongest changes observed for pores ranging in size from <2 to 50 nm. Important factors influencing the structure and dynamics of confined fluids include the average pore size and pore size distribution, the degree of pore interconnection, and the character of the liquid–surface interaction. The confining matrices of interest to earth and materials sciences usually contain oxide structural units and thus are hydrophilic. The pore size distribution and the degree of porosity and inter-connection vary greatly amongst porous matrices. Rocks typically possess irregular porous structures, whereas zeolites, and layered systems, for instance clays, have high degrees of internal order. In clays, the interlayer distance may depend on the level of hydration. The properties of neutrons make them an ideal probe for comparing the properties of bulk fluids with those in confined geometries. In this presentation, we provide an overview of research performed on fluids confined in materials of interest to the earth and material sciences (silicas, aluminas, zeolites, clays, rocks, etc.) emphasizing those techniques that assess both structural modification and dynamical behavior such as small-angle (SANS) and quasielastic neutron scattering (QENS). Molecular dynamics (MD) simulations will be described that provide atomistic characterization of the confined fluid behavior as well as aid in the interpretation of the neutron scattering results.