

Subject: Predominance Diagrams for Americium, Neptunium and Thorium in Reacted GW Brine

Predominance diagrams were generated for americium, thorium and neptunium to serve as representative cases for the +III, +IV and +V actinides in reacted GW Brine using the Sandia National Laboratories FMT_050405.CHEMDAT thermodynamic database for the relevant chemical species and their associated thermodynamic values, including Pitzer parameters for calculations at high ionic strength.

The pH vs. E_h diagrams were generated as follows: For the brine composition, the GW Brine After Reaction with MgO, Halite and Anhydrite case (Brush 2005a) was used as the base concentration set for the thermodynamic calculations using Woolery's EQ36 package. The actinide solubilities, using americium for An(III), thorium for An(IV) and neptunium for An(V), were taken from FMT run #8 (see Table 5, PABC-2005) and the parameters from that specific run, e.g. $\log f(\text{CO}_2) = -5.5$, solution density = 1.23 g/cc, etc. were used to complete the boundaries of the calculation. Since there was no redox dependency in the Sandia thermodynamic dataset, the pH was varied at constant E_h and the speciation thereby determined to generate the overall dependency on the pH axis. The water stability boundaries, i.e. maximum and minimum E_h values for any given pH, were calculated by holding pH constant and varying E_h to determine the fugacity = 1 atmosphere points for O_2 and H_2 .

Program ACT2 of The Geochemist's Workbench suite of programs was used to generate a template E_h versus pH plot for each actinide and Photoshop CS was then used to adjust the plot to reflect the EQ36 Pitzer parameter calculation.

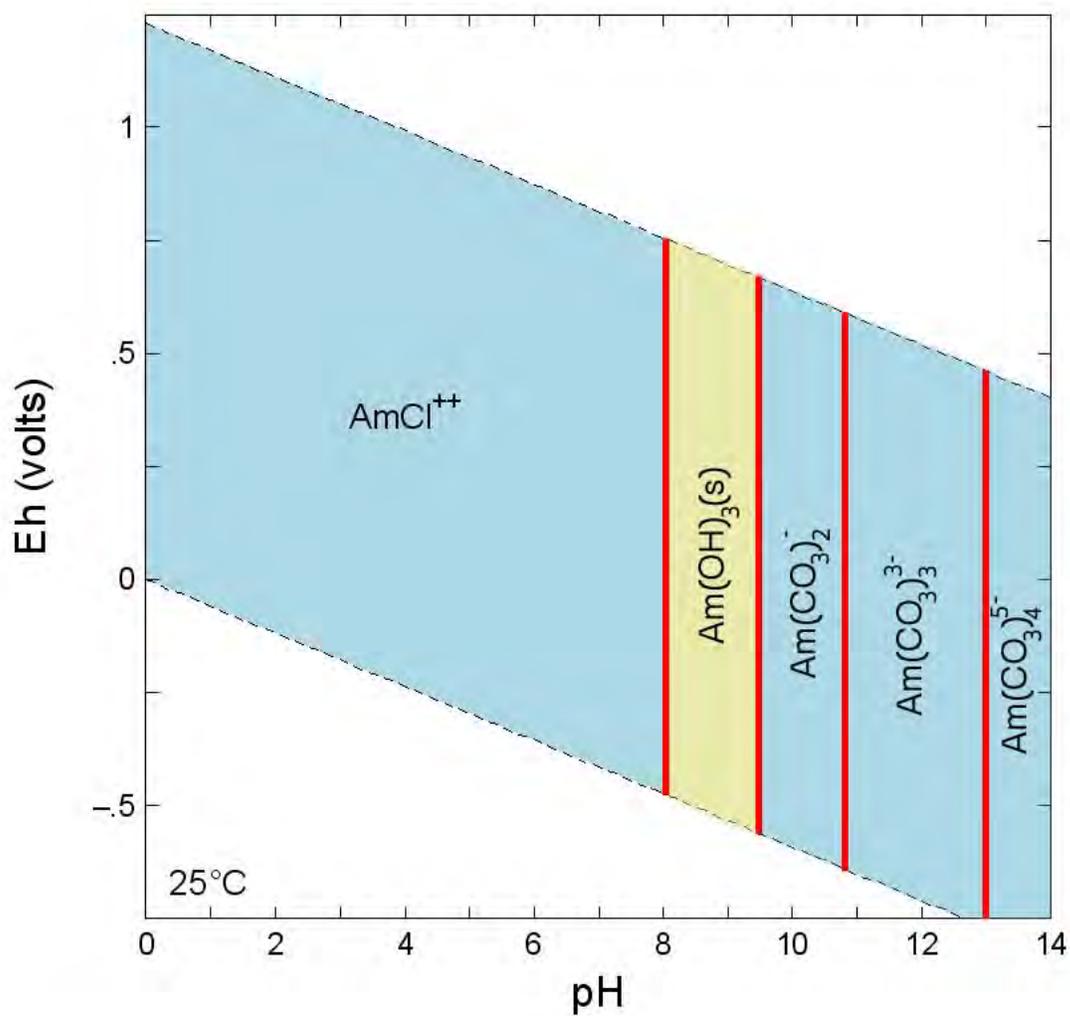


Figure 1 Eh versus pH diagram for americium(III).

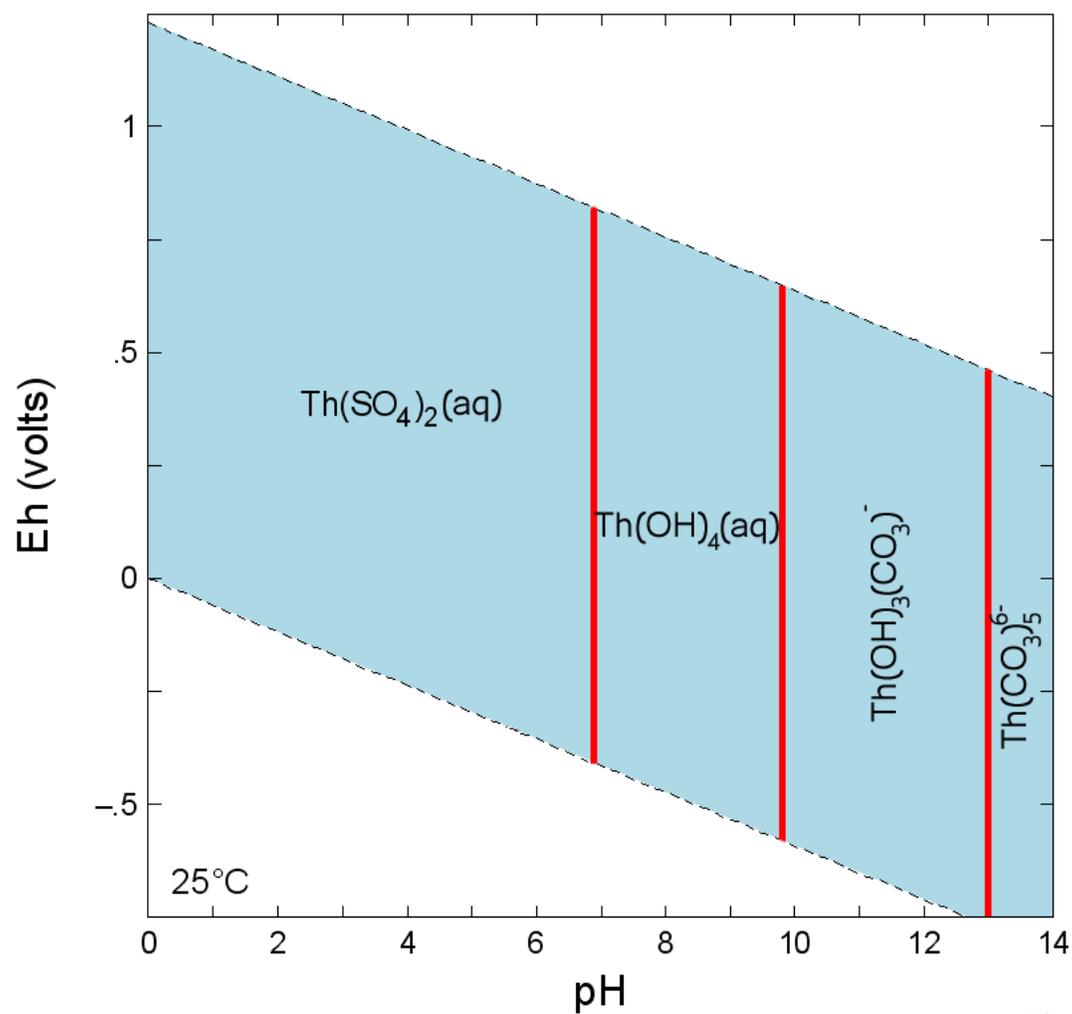


Figure 2 E_h versus pH diagram for thorium(IV).

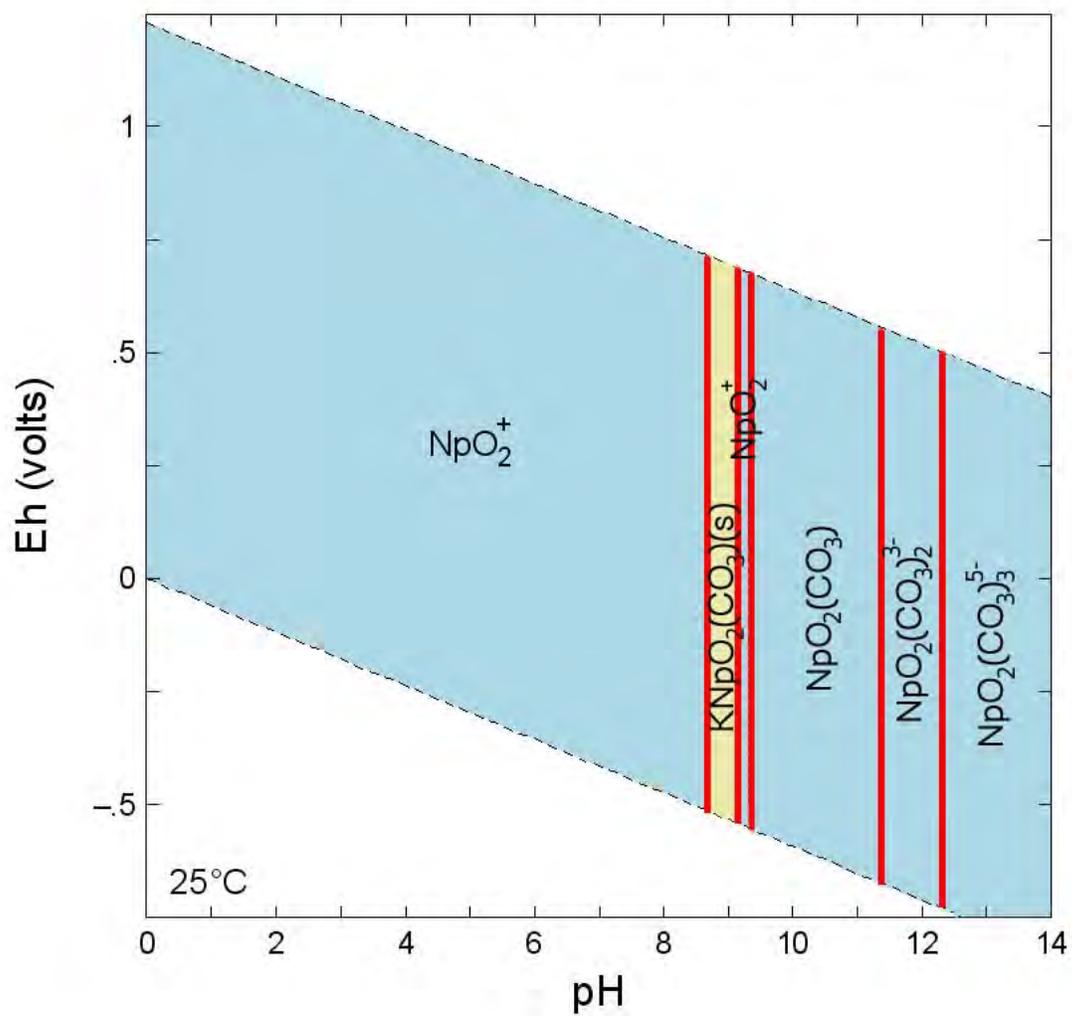


Figure 3 E_h versus pH diagram for neptunium(V).