Alicia Mullins

From: David Pickett
Sent: Tuesday, February 13, 2007 6:50 PM
To: spainter@swri.edu
Subject: RE: possible paper of interest ?
Attachments: colloid surface area calculations.xls

Follow Up Flag: Follow up
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Yes, looks relevant.

I've attached a spreadsheet showing some possibly useful calculations I did the last time we talked about all this. Main points: note specific SA with colloid diameter; note mass fractions and bulk specific SA given a flat size distribution based on counts. IF (IF!) we could say something about size distribution of "fresh" corrosion product colloids, we could say something about bulk specific SA. It is very low in my examples, because so much of the mass is in the large colloids.

This, of course, ignores secondary surface area effects on colloid surfaces - which will lower bulk specific SA. So, maybe not useful.

David

-----Original Message-----
From: Scott Painter [mailto:spainter@swri.edu]
Sent: Tuesday, February 13, 2007 5:23 PM
To: 'dpickett@swri.org'
Subject: possible paper of interest ?

The full paper is at http://www.nea.fr/html/science/docs/pubs/nea3054/nea3054-poster-session.pdf.

XAFS INVESTIGATION OF LANTHANIDE SORPTION ONTO FERRIHYDRITE AND TRANSFORMATION PRODUCTS BY TEMPERING AT 75°C

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Abstract
The time-dependent changes of Lu speciation, initially sorbed onto hydrous ferric oxides (HFO) during tempering (75°C) and leading to stable crystalline transformation product hematite, is studied. Three-step sequential extraction ($MgCl_2$, oxalate/oxalic acid; dithionite-citrate-bicarbonate) of the solid material shows that the amount of Lu extracted with crystalline Fe-phases (Fe_D) increases with ageing time. Extended X-ray absorption fine structure (EXAFS) study reveals a shortening of the Lu-O bond distance and an increase of the asymmetry of the first shell contribution in the Fourier transform with increasing tempering time. Both EXAFS and the extraction study show that Lu(III), an actinide analogue, is likely incorporated into the Fe oxide phase during transformation.

Colloid Specific Surface area calculations

Assume Spherical. Density = 3.5 g/cc.

Colloid diameter (nm)	Surface area (m2)	Volume (m3)	mass (g)	Specific SA (m2/g)
1	3.14E-18	5.24E-28	1.83E-21	1714
5	7.85E-17	6.54E-26	2.29E-19	343
10	3.14E-16	5.24E-25	1.83E-18	171
100	3.14E-14	5.24E-22	1.83E-15	17.1
1000	3.14E-12	5.24E-19	1.83E-12	1.71
6	1.13E-16	1.13E-25	3.96E-19	285.71
50	7.85E-15	6.54E-23	2.29E-16	34.29
200	1.26E-13	4.19E-21	1.47E-14	8.57
450	6.36E-13	4.77E-20	1.67E-13	3.81

Assume a loguniform, discrete size distribution

Colloid diameter (nm)	number fraction	mass fraction	Composite Specific SA (m2/g)
1	0.25	9.99E-10	1.73E+00
10	0.25	9.99E-07	
100	0.25	9.99E-04	
1000	0.25	9.99E-01	

Assume TSPA-SR colloid size distribution, discrete

Colloid diameter (nm)	cumul prob, colloid size	proportion colloids at size	mass fraction	Composite Specific SA (m2/g)
1	0			
6	0.2	0.2	2.15E-06	4.36E+00
50	0.4	0.2	1.25E-03	
100	0.6	0.2	9.98E-03	
200	0.8	0.2	7.98E-02	
450	1	0.2	9.09E-01	