## LSNReviews

**From:** David Pickett [dpickett@gargol.cnwra.swri.edu]
**Sent:** Wednesday, March 07, 2001 3:42 PM
**To:** 'Vladimir Cvetkovic'
**Cc:** 'David Turner (dturner)'
**Subject:** RE: Los Alamos colloid study
**Attachments:** zz_sep_158079.xls

**Follow Up Flag:** Follow up
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Vladimir,

Here's what I did. As it turns out, I did not have to make any assumptions in order to go from Kd to percent sorbed. (However, see below regarding container sorption.)

Define:
mc = mass (or activity) of Pu on colloids ms = mass (or activity) of Pu in solution gc = mass of colloids in system vs = volume of solution (ml) C = colloid concentration = gc/vs (g/ml) = 0.0002 g/ml (= 200 mg/L)

Kd = (mc/gc)/(ms/vs)
= (mc/ms)/C
ms/mc = 1/(Kd*C)

% sorbed = 100*(mc/(mc + ms))
= 100/(1 + ms/mc)
= 100/(1 + (1/(Kd*C)))

The resulting values for percent sorbed for the columns of data in the file are below my message. Or, look at the attached Excel file.

You will notice that these values don't correspond exactly with what's on Figure 1 in LA-UR-00-5121. I believe that is due to the fact that they accounted for sorption to the surfaces of the sample tube (see p 12). They make this correction in calculating Kd with Eqn 5, but I would guess that there was no correction made for percent sorbed. In other words, the value on Figure 1 is straight from the experiments; in each case, some of the remaining Pu is in solution, and some is on surfaces.

These differences may not be important for your purposes, but you may want to see how they compare visually. My calculation of % sorbed may be more "true," in that it is derived from a Kd for which container sorption was corrected out.

David

50.0
72.2
82.1
93.8
95.1
95.7
96.3
96.3
96.8
97.1
99.3
96.0

4.4
8.3
14.2
16.7
44.4
53.7
4.6
4.8
18.0
19.4
25.4
56.5
1.7
25.4
52.4
53.7
57.3
61.8
55.0
60.3
66.4
66.4
70.6
75.0

> -----Original Message-----
> From: Vladimir Cvetkovic [mailto:vdc@avat09.ce.kth.se]
> Sent: Wednesday, March 07, 2001 11:26 AM
> To: David Pickett
> Cc: David Turner (dturner)
> Subject: RE: Los Alamos colloid study
>
>
> david --
>
> thanks for the data files. As I indicated earlier, I need the percent
> Pu vs time. I didnt really figure out how they infer their Kd.
> You mention
> eq. 5 with a few assumptions; can you say which assumptions you have
> to make, i.e. can you specify how to get the percent Pu from their Kd
> at a given time? Thanks!
>
> Vladimir
>
>
> On Wed, 7 Mar 2001, David Pickett wrote:
>
> > Vladimir,
> >
> > Among the available online DOE data, I found separate data
> files for the
> > Figure 1 plot and for the Table 16 data. They are attached
> as text files.
> > It doesn't appear that they did the kinetics experiment at
> several colloid
> > concentrations. It is possible that there may be something

> from the earlier
> > LANL report we gave you (LA-UR-98-3057) that would provide
> a comparison.
> > The latter report has several sets of kinetic experimental
> data. Let me
> > know if you want data files for those; I probably have them now.
> >
> > By the way, the Figure 1 data (from LA-UR-00-5121) on the
> file are reported
> > only as Kd, rather than as percent sorbed--as in the
> figure. I did a simple
> > calculation trying to reproduce the percent numbers, using
> equation 5, and
> > making a couple of assumptions. I came pretty close to
> what's on the
> > figure--close enough that I am sure they are the appropriate data.
> >
> > David
> >
>

S00189_001 Data Report
DTN LA0003NL831352.002

| ROW | TIME h | WATER | COLLOIDS | PLUTONIUM SORPTION DISTRIBUTION COEFFICIENT mL/g | Kd, ml/g | assume C(coll) = 200 mg/L = 0.0002 g/ml<br>calculated % sorbed |
|---|---|---|---|---|---|---|
| *** | ********** | ********** | ********** | ********** | | |
| 1 | 1 | J13 | Hematite | (5.0 +/- 0.05) x 10^3 | 5.00E+03 | 50.0 |
| 2 | 4 | J13 | Hematite | (1.3 +/- 0.07) x 10^4 | 1.30E+04 | 72.2 |
| 3 | 24 | J13 | Hematite | (2.3 +/- 0.1) x 10^4 | 2.30E+04 | 82.1 |
| 4 | 48 | J13 | Hematite | (7.5 +/- 0.7) x 10^4 | 7.50E+04 | 93.8 |
| 5 | 96 | J13 | Hematite | (9.7 +/- 1.7) x 10^4 | 9.70E+04 | 95.1 |
| 6 | 240 | J13 | Hematite | (1.1 +/- 0.03) x 10^5 | 1.10E+05 | 95.7 |
| 7 | 1 | SYN.J13 | Hematite | (1.3 +/- 0.03) x 10^5 | 1.30E+05 | 96.3 |
| 8 | 4 | SYN.J13 | Hematite | (1.3 +/- 0.05) x 10^5 | 1.30E+05 | 96.3 |
| 9 | 24 | SYN.J13 | Hematite | (1.5 +/- 0.2) x 10^5 | 1.50E+05 | 96.8 |
| 10 | 48 | SYN.J13 | Hematite | (1.7 +/- 0.0) x 10^5 | 1.70E+05 | 97.1 |
| 11 | 96 | SYN.J13 | Hematite | (7.0 +/- 0.03) x 10^5 | 7.00E+05 | 99.3 |
| 12 | 240 | SYN.J13 | Hematite | (1.2 +/- 0.3) x 10^5 | 1.20E+05 | 96.0 |
| 13 | 1 | J13 | Montmorillonite | onite (2.3 +/- 0.2) x 10^2 | 2.30E+02 | 4.4 |
| 14 | 4 | J13 | Montmorillonite | onite (4.5 +/- 1.5) x 10^2 | 4.50E+02 | 8.3 |
| 15 | 24 | J13 | Montmorillonite | onite (8.3 +/- 0.8) x 10^2 | 8.30E+02 | 14.2 |
| 16 | 48 | J13 | Montmorillonite | onite (1.0 +/- 0.03) x 10^3 | 1.00E+03 | 16.7 |
| 17 | 96 | J13 | Montmorillonite | onite (4.0 +/- 0.7) x 10^3 | 4.00E+03 | 44.4 |
| 18 | 240 | J13 | Montmorillonite | onite (5.8 +/- 1.1) x 10^3 | 5.80E+03 | 53.7 |
| 19 | 1 | SYN.J13 | Montmorillonite | onite (2.4 +/- 0.3) x 10^2 | 2.40E+02 | 4.6 |
| 20 | 4 | SYN.J13 | Montmorillonite | onite (2.5 +/- 0.6) x 10^2 | 2.50E+02 | 4.8 |
| 21 | 24 | SYN.J13 | Montmorillonite | onite (1.1 +/- 0.3) x 10^3 | 1.10E+03 | 18.0 |
| 22 | 48 | SYN.J13 | Montmorillonite | onite (1.2 +/- 0.02) x 10^3 | 1.20E+03 | 19.4 |
| 23 | 96 | SYN.J13 | Montmorillonite | onite (1.7 +/- 0.09) x 10^3 | 1.70E+03 | 25.4 |
| 24 | 240 | SYN.J13 | Montmorillonite | onite (6.5 +/- 2.4) x 10^3 | 6.50E+03 | 56.5 |
| 25 | 1 | J13 | Si.PST-1 | (8.6 +/- 3.6) x 10^1 | 8.60E+01 | 1.7 |
| 26 | 4 | J13 | Si.PST-1 | (1.7 +/- 1.1) x 10^3 | 1.70E+03 | 25.4 |
| 27 | 24 | J13 | Si.PST-1 | (5.5 +/- 0.1) x 10^3 | 5.50E+03 | 52.4 |
| 28 | 48 | J13 | Si.PST-1 | (5.8 +/- 0.1) x 10^3 | 5.80E+03 | 53.7 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 29 | 96 | J13 | Si.PST-1 | (6.7+/- 0.03) x 10^3 | 6.70E+03 | 57.3 |
| 30 | 240 | J13 | Si.PST-1 | (8.1 +/- 0.1) x 10^3 | 8.10E+03 | 61.8 |
| 31 | 1 | SYN.J13 | Si.PST-1 | (6.1 +/- 0.2) x 10^3 | 6.10E+03 | 55.0 |
| 32 | 4 | SYN.J13 | Si.PST-1 | (7.6 +/- 0.3) x 10^3 | 7.60E+03 | 60.3 |
| 33 | 24 | SYN.J13 | Si.PST-1 | (9.9 +/- 0.4) x 10^3 | 9.90E+03 | 66.4 |
| 34 | 48 | SYN.J13 | Si.PST-1 | (9.9 +/- 0.5) x 10^3 | 9.90E+03 | 66.4 |
| 35 | 96 | SYN.J13 | Si.PST-1 | (1.2 +/- 0.004) x 10^4 | 1.20E+04 | 70.6 |
| 36 | 240 | SYN.J13 | Si.PST-1 | (1.5 +/- 0.6) x 10^4 | 1.50E+04 | 75.0 |