HLWYM HEmails

From: David Pickett
Sent: Thursday, March 01, 2007 12:13 PM
To: Tae Ahn; Yi-Ming Pan; Xihua He; Scott Painter; Hakan Basagaoglu
Cc: english.pearcy@swri.org; Osvaldo Pensado
Subject: Chromium in in-package chemistry and colloids

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All,

In looking at parameters yesterday, I came across the fact that, as of Rev 04 of the in-package chemistry abstraction report (ANL-EBS-MD-000037), DOE no longer allows chromium to be in the Cr(VI) oxidation state. Rather, they force EQ3/6 to use only Cr(III) species. They have recognized the weakness of the Cr(VI) assumption and that it "leads to artificially high ionic strengths." This has implications for their modeled colloid release.

I mention this because I'd made an issue of this in our discussions and documents, before I'd seen Rev 04. (Tae: Cr is mentioned in the Review strategy.) Their approach to Cr chemistry now appears reasonable.

Figures 6-7, 6-8, 6-14, and 6-15 of the report show the dominant aqueous species. Those that are most prominent, and thus contribute most to ionic strength, are Ni++, MoO4--, and NO3-. I haven't paid attention to these in the past. For the long term in all models, ionic strength appears to be heading to values near or below DOE's colloid stability limit of 0.05 M (see also Figure 6-9). Note that they don't use these time-dependent chemical models in TSPA - they're used just to set the ranges.

Bottom line:

1. If DOE stays with this Cr approach, I don't have questions for them. It would probably be good to at least ask if they're sticking with it.
2. Colloid release in TSPA _may_ be higher overall if model ionic strengths do get below 0.05 M. I haven't yet looked at their abstraction in detail to see what ionic strengths would result (pp 8-3 and 8-4). It depends only on liquid flux.

David

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