HLWYM HEmails

From: Richard Codell
Sent: Wednesday, March 07, 2007 9:03 PM
To: Osvaldo Pensado; Christopher Grossman
Cc: James Myers; James Winterle; Roberto Pabalan; Andy Campbell
Subject: RE: Fwd: Reference needed on diffusion coefficient from Codell

Osvaldo:

Thanks for the explanation. I am glad that you and Bobby gave it a lot of thought, but I was unaware of the rationale behind the TPA implimentation of the corrosion chemistry and hadn't been aware of the scientific notebook. I have not been up to speed on what has been happening in the corrosion and chemistry area.

I did a little checking on the files I had available to me and found that in fact the coding you present was mine. I cannot recall how it came about though, but I am sure its in my notes back in Rockville.I looked at the Chem Eng handbook and the Handbook of Chem and Physics and didn't see it thee. The date I had for it in my annotation and comments was 7/23-25/2002. You may be able to find it in an SCR about that time. Otherwise, I will get you the information the next time I am in Rockville. I may try to be there at the end of March to take part in the validation meeting, but I don't know yet.

Dick

>>> Osvaldo Pensado <opensado@cnwra.swri.edu> 3/7/2007 4:10 PM >>>
Thanks Dick,

With respect to the observation on the chemistry, the data (Pabalan's speciation computations) point at weak correlations among other ions than chloride, bicarbonate, hydrogen. I did testing on the corrosion equations adopting the whole correlation matrix and I found approximately the same frequency of localized corrosion than for cases where only strong correlations were implemented. This test was only documented in a scientific notebook supporting the report "Passive and Localized Corrosion of Alloy 22 --Modeling and Experiments, CNWRA 2005-02."

Therefore, for the sake of simplicity, we dropped the weak correlations
(<0.5) and preserved only the strong correlations in the TPA sampling.

Pabalan and I discussed that there was nothing that could prevent other ionic compositions to be established. We thought it was reasonable to do sampling (preserving only the strong correlations) to construct "feasible" solution compositions. We intended to encompass other water chemistries than those drawn with few thermodynamic simulations (from which the correlation matrix was computed). By the way, the LC frequency using only the few thermodynamic simulations (i.e., considering only real water
compositions) was less than in the extended approach considering "feasible"
water compositions (i.e., sampled water compositions). Again, I documented this in the scientific notebook previously referred.

We are looking at the thermodynamic simulations again. We are revising the distributions. Preliminary results indicate that there is only one strong correlation (pH and bicarbonate). We may need to revise the distribution functions during TPA validation testing.

Thanks also for looking at the reference on the temperature dependence of the diffusion coefficient. Our records indicate R. Codell as the originator of the diffusive release model (although we may have indeed edited the code). We will look at the SCR and see if there is any reference.
Otherwise, we will do as best as we can to document the diffusion model.

Thanks again Dick.

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-----Original Message-----
From: Richard Codell [mailto:RBC@nrc.gov]
Sent: Wednesday, March 07, 2007 1:47 PM
To: Osvaldo Pensado; Christopher Grossman
Cc: Andy Campbell
Subject: Re: Fwd: Reference needed on diffusion coefficient from Codell

Sorry, I didn't respond immediately and I lost track of this email. It may
have something to do with dementia.

I only vaguely remember where those equations originated, but I am almost
sure it was a textbook, probably one on physical chemistry or transport
phenomena. I seem to recall that the diffusion correction factors came out
of the Handbook of Chemistry and Physics or maybe the Chem Engr Handbook.
Its likely that the history of this thing is in my notes on diffusion models
or on the releaset code in the file, but I don't have these files here. I
beleive that I would have given the reference in a Software Change Report
dating from that time, probably around 2001 or before. I am not exactly sure
that I coded those lines in releaset myself. I looked at the lines and its
not really my style; for example, it has 293 -273 explicitly on lines 2741
and 2742. That doesn't look like something I would do. Also, I tend to group
the denominator in parentheses to prevent ambiguity. Therefore, its possible
that someone else coded this or maybe just changed what I wrote. You might
check with George Adams or Ron Janetzke.

I will do what I can here, in terms of what I might have electronically.
Earlier versions of the code, memos and notes, but all my files on diffusion
are in Rockville. I will probably be back before long, maybe in May,

and if
all else fails, I can look through my notes at that time.

On another matter, thanks for the quick response to my questions on the TPA
revisions. I am generally satisfied with the response, especially because I
recognize the limitations we all have to work under for making big changes
to the TPA code and philosophy. I am interested wherever possible to ward of
criticism of our models by asking obvious questions about the defensibility
of assumptions. In this regard, I am still a little concerned about the
assumptions of chemistry for corroding the waste packages. Do the chemical
data support the assumption that most of the ionic strengths are
uncorrelated, and can therefore be sampled independently? I seem to recall
that the DOE data collection and speciation modeling came up with a variety
of waters. Each water type had a fixed concentration of each ionic species.
Taking these simulations and data and coming up with a distribution of each
species that can be sampled independently (except for the case of the
carbonate/pH correlation) seems to be a bit of a stretch from the initial
supporting information. It may be that I am missing something, and perhaps
there is a DOE or Center report supporting this idea, but I am not aware of
it. Therefore I am bringing it to your attention because its an obvious
question that someone might have, and we should be prepared to defend the
model.

Keep me posted on the validation efforts and what I can do to contribute.
Should I plan to attend one of the meetings in person?

Sincerely
Dick

>>> Christopher Grossman 2/28/2007 12:32 PM >>>
Dick-

Osvaldo is looking for a reference for your implementation of the diffusion
model. Take a look at the attachment for more details and a refresher on
the issue and let me know what the reference is for the particular
equations, if any.

Chris

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>>> Osvaldo Pensado <opensado@cnwra.swri.edu> 02/28/2007 12:30 PM >>>

Chris,

I am looking for a reference for the diffusion model to be described in the
user manual. I browsed the code and I pulled the diffusion equations. I
understand the assumptions and we can take care of describing the concepts.

However, Dick implemented a complex equation for the temperature dependence
of the diffusion coefficient of radionuclides in water. We need a reference
for that equation. Could you please share the attachment with Dick to refresh his memory?

Thanks

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Created By: Richard.Codell@nrc.gov

Recipients:
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Tracking Status: None
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