From: Roberto Pabalan
Sent: Friday, August 17, 2007 4:22 PM
To: Miriam Juckett
Cc: James Myers
Subject: FW: Temperature Range Validation of Pitzer Database

Miriam,

As Jim indicated, DOE conducted model validation up to 140C. I looked at the comparison of experimental and calculated values documented in section 7 of the AMR. In general, the experimental and calculated values are in good agreement.

If there is still some question regarding the DOE model validation, we can discuss it when I get back in the office on August 20.

--Bobby

-----Original Message-----
From: Jim Myers [mailto:jmyers@swri.edu]
Sent: Friday, August 17, 2007 2:54 PM
To: 'Bobby Pabalan'
Subject: FW: Temperature Range Validation of Pitzer Database

James L. Myers, Ph.D.
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-----Original Message-----
From: Jim Myers [mailto:jmyers@cnwra.swri.edu]
Sent: Thursday, August 16, 2007 3:47 PM
To: 'miriam.juckett@gmail.com'
Subject: Temperature Range Validation of Pitzer Database

Miriam,

The DOE did essentially validate the model and consequently the Pitzer data base over the 25C to 140C temperature range. This is discussed in sections 7.1.1.2 and 7.1.2 and presented in Figures 7-3 to 7-53. Their requirement is that the model match the data within a factor of 10 (aka 1 order of magnitude).

The exceptions are discussed on p 7-25 and included below.

> Except for two cases, all predictions are within a factor of 10 of the measurements (in accordance with model validation criteria shown in Table 7-1) and are usually within a factor of 3. One exception is the underprediction of Na solubility in the Na-Ca-NO_3 system (Figure 7-40). The total nitrate and calcium concentrations are within the range of measurements but the sodium concentration is far below measurements. The other exception is the

$Cl:NO_3$ ratio in the $Mg\text{-}Cl\text{-}NO_3$ system (Figure 7-53). The model underpredicts this ratio by more than a factor of ten at 20°C. These two systems have predicted RH_d values between 4% and 30%.

The uncertainties that appear in the comparisons are captured and propagated into model uncertainty estimates in Section 7.5. Potential model bias as it might relate to conservatism is also addressed in Section 7.5.

The question that I have is how do you capture and propagate variable uncertainty or model bias (when the model bias varies)? For example they have a criteria of +/- a factor of 10. How do you capture and propagate the uncertain for those systems/species that don't meet the criteria?

Just looking at the figures it appears that the model fit is poorer at higher temperature, but it is within their factor of 10 criteria so they don't analyze or evaluate it.

Let me know if you have any additional questions.

Jim

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Subject: FW: Temperature Range Validation of Pitzer Database
Sent Date: 8/17/2007 4:21:51 PM
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From: Roberto Pabalan

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Recipients:
"James Myers" <jmyers@cnwra.swri.edu>
Tracking Status: None
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Tracking Status: None

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