HLWYM HEmails

From: Bret Leslie
Sent: Thursday, September 04, 2008 7:49 AM
To: junli@unc.edu
Cc: Bret Leslie
Subject: FW: availability of TPA 5.1 user guide and TPA5.1a code
Attachments: Question regarding the glass dissolution model in TPA5.1.doc

Jun,

Thanks for your comment. I have passed on your information to the staff at the Center for Nuclear Waste Regulatory Analyses, for their consideration. If NRC updates the TPA code we will consider the information that is available at that time. Please note that DOE provided revision 2 of ANL-EBS-MD-000016 as a reference supporting their license application. We appreciate you pointing out the different approaches, and rates that are derived from the different versions of the Defense HLW Glass Degradation Model Report.

Cheers,

Bret

From: Jun Li [mailto:junli@unc.edu]
Sent: Thursday, August 28, 2008 6:14 PM
To: Bret Leslie
Cc: junli@unc.edu
Subject: RE: availability of TPA 5.1 user guide and TPA5.1a code

Dear Mr. Bret Leslie:

How are you doing?

Thanks again for your help to get the TPA5.1 code.

I am working on glass form waste issue recently where the glass form waste dissolution model is used. The default parameters included in the TPA5.1 package seems to be out of date. Please see the attached document for the details.

Please knowledge me if I am wrong.

Thanks.

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From: Bret Leslie [mailto:BWL@nrc.gov]
Sent: Monday, October 08, 2007 7:44 AM
To: jli7@ncsu.edu
Cc: Sitakanta Mohanty; yim@ncsu.edu; Bret Leslie; Christopher Grossman
Subject: availability of TPA 5.1 user guide and TPA5.1a code

Dear Dr. Li,

I received your inquiry about obtaining the "new" version of the TPA code. Dr. Mohanty's reply to you on the newness of the code was correct. Total-system Performance Assessment (TPA) Version 5.1a was made publicly available October 4, 2007.

A new version of the TPA code (5.1a) and a user guide has been made publicly available through the U.S. Nuclear Regulatory Commission Agencywide Documents Access and Management System (ADAMS). ADAMS is accessible thru the internet at http://www.nrc.gov/reading-rm/adams.html, and the ADAMS accession numbers, i.e., "MLxxxxxxxxx, for the user guide and code are ML072710060, and ML072770577, respectively. I should note that the user guide is .pdf file and will be downloadable. The code itself is on a CD-ROM, which I will transmit to you via letter, later this week or early next week. At that time I will also enclose a CD-ROM copy of the user guide.

The TPA Version 5.1a computer code was developed through a joint effort between the NRC and the Center for Nuclear Waste Regulatory Analyses (CNWRA) staff. TPA Version 5.1a is a review tool developed to assist staff in prelicensing activities and reviewing a potential U.S. Department of Energy license application.

I also wanted to inform you that NRC staff will be discussing TPA Version 5.1a in an upcoming public meeting. NRC staff will brief the Advisory Committee on Nuclear Waste and Materials (ACNW&M) in Rockville, Maryland at their 183rd Meeting on the morning of October 17, 2007. More information on the ACNW&M meeting is available at http://www.nrc.gov/reading-rm/doc-collections/acnw/agenda/2007/183.pdf.

If I can be of further assistance, please let me know.
Bret Leslie, Senior Project Manager

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Subject: FW: availability of TPA 5.1 user guide and TPA5.1a code
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Created By: Bret.Leslie@nrc.gov

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Question regarding the glass dissolution model in TPA5.1.doc		135232

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Question regarding the glass dissolution model in TPA5.1

The glass dissolution model described in the TPA5.1 user's guide (page 10-22):

$$r_g = k_o 10^{\eta pH} exp\left(-\frac{E_{ag}}{RT}\right) \quad (10\text{-}9)$$

where

r_g	—	glass waste form dissolution rate [g/m^2/day]
k_o	—	intrinsic dissolution rate [g/m^2/day]
η	—	pH dependence coefficient [unitless], as specified by the *tpa.inp* parameter pHParameterLowRange[] or pHParameterHighRange[]
pH	—	pH of the in-package water [unitless], as specified by the *tpa.inp* parameter pHForGlassModel[]
E_{ag}	—	effective activation energy [kJ/mol/K], as specified by the *tpa.inp* parameter GlassActivationEnergyLowRange[kJ/mol-K] or GlassActivationEnergyHighRange[kJ/mol-K]
R	—	ideal gas constant [8.314 J/(mol K)]

The parameter k_o is specified in *tpa.inp* as $\log_{10}(k_o)$ via the parameters LogOfGlassDissolutionConstantHighRange[] and LogOfGlassDissolutionConstantLowRange[], with k_o in units g/m^2/day. The "LowRange" and "HighRange" parameters, identified above, are selected when the value of the *tpa.inp* parameter pHForGlassModel[] is less than or greater than six, respectively (Bechtel SAIC Company, LLC, 2001).

Figure 1 snapshot picture from TPA5.1 User's Guide (page 10-22)

The default values in "tpa.inp" for $\log_{10}(k_0)$ are:

uniform
LogOfGlassDissolutionConstantHighRange[]
4.708618, 5.708618

uniform
LogOfGlassDissolutionConstantLowRange[]
6.308618, 8.308618

It seems those values are referred from Bechtel SAIC 2001 report. I only can find one version of the Bechtel SAIC 2004 report with same title as "Defense HLW Glass Degradation Model", ANL-EBS-MD-000016 REV 01 ICN01F, February 2004. Page 108 of this report shows different values for the parameter k_0 :

$$rate_G = k_{E_acidic} \times 10^{-0.49 \cdot pH} \times exp(-31/RT) \quad \text{(Eq. 40a)}$$

$$rate_G = k_{E_alkaline} \times 10^{0.49 \cdot pH} \times exp(-69/RT) \quad \text{(Eq. 40b)}$$

Different triangular distributions are used for k_E in acidic and alkaline solutions. Values for k_{E_acidic} and $k_{E_alkaline}$ to be used for any time step in a realization are selected from the following distributions:

The maximum value of k_{E_acidic} is 1.15×10^7 g/(m^2·d).
The minimum and most probable value of k_{E_acidic} is 8.41×10^3 g/(m^2·d).
The maximum value of $k_{E_alkaline}$ is 3.47×10^4 g/(m^2·d).
The minimum and most probable value of $k_{E_alkaline}$ is 2.82×10^1 g/(m^2·d).

Figure 2 Snapshot picture from Bechtel SAIC 2004 report (page 108)

So two questions exist:

1) the recommended value for k_0 is different from TPA5.1 and Bechtel SAIC 2004 report
2) The pH value to distinguish low or high range is 6 in TPA5.1 and 7 in Bechtel SAIC 2004 report.

For question 2), as pH value for pure water is "7", "7" sounds more reasonable for the standard to distinguish low or high range. And "7" is also used as the standard in the source code "releaset.f".

For question 1), I did a trial calculation which used mean value of k_0 from TPA5.1 and the most probable value of k_0 from Bechtel SAIC 2004, the result is shown in table 1.

Table 1 Trial calculation of rate_g

	Value from TPA5.1	Value from Bechtel SAIC 2004
k0 [g/m^2/day]	2.04E+07	8.41E+03
r_g [g/m^2/day]	1.37E+00	5.68E-04
	pH=5, T=343K,Eag=31KJ/mol-K	

The resulted value of r_g using k_0 value from Bechtel SAIC 2004 report is much closer to the published glass dissolution rate (~10^-3 [g/m^2/day] at the same condition, Knauss et al, "Dissolution Kinetics of a Simple Analogue Nuclear Waste Glass as a Function of pH, Time and Temperature", Mat. Res. Soc. Symp. Proc. Vol. 176, p. 371-381, 1990)

So, two suggestions:

1) The statement in the TPA5.1 user's guide regarding the pH value to distinguish low or high range of glass dissolution model should be changed from "6" to "7"
2) The default value of parameter k_0 in the "tpa.inp" should be updated to newer values.