HLWYM HEmails

From: Richard Codell
Sent: Tuesday, August 26, 2003 6:22 PM
To: Ronald Janetzke; Sitakanta Mohanty
Cc: Andy Campbell; David Esh; Timothy McCartin
Subject: releaset review

I have reviewed the problems you encountered in releaset and will address them the best I can.

1. I found one coding error. The code inadvertently corrects the total radionuclide in the waste for the gap fraction in the glass model. In subroutine liqrel, the loop beginning with "do 410 k=1,nchns" should be bypassed for the glass model (imodel=5). This accounted for a small removal of the radionuclides from the solid glass mass. It had a small effect on the release rate and cumulative release from the waste package.

2. I was unable to see the big discrepency for the glass model with Tc-99 release. I set up the following problem:

-Tc99 only
-time-varying temperature
-2 initially failed waste packages
-time-varying flow rate into and out of package -flow-through model -pH glass = 8.40195
-Log(Keff) = 6.9 = 7.443e6 g/m2/day
-eta-high = 0.4
-E-high = 80 kJ/mol

The cumulative release from the fuel and the wp was very close - 95.345 Ci for glass from the subarea and 96.471 Ci from the waste packages for the subarea. When I fixed the temperature at 110 C, the results were similar.

I would not expect the release rate from the fuel and the release rate from the WPs to be identical because even though its the flow-through model, the volume is adjusted so that there is a time constant of between 20 and 50 years to help the numerical calculations work faster. The highest release rate from the WP is lower than the release rate from the glass because of this smoothing. Like I say, I did not seem to encounter any serious problem with the glass model, but I could not follow all that you did. If you could get me the exact conditions for your test, I might have an easier time finding any problem areas for the glass model.

3. I agree with your corrections to the program for the mass balance of the fuel.

4. I agree with a change in the enthalpy to -50.46 kJ/mol in the schoepite model (model 4)

5. I agree with your change to the logic for the schoepite model that inadvertently set the release rate to zero.

6. I do not agree that the wetted fraction should be included in the schoepite model, since this model relies on the total uranium solubility limit and should not be a function of exposed surface area. I believe this is the source of the error for the non-zero release rate of U-238 when leaching rate was zeroed out for model 4, since the code does not check for exposed surface area when model 4 is used. It is not an important point however since the release rate from model 4 is always so small. I could not follow exactly the test you did for this model, so I cannot be sure I understand all you are saying in the report.

7. The unzipping model is in the code, but it can either be used or ignored. The parameters allow an entire range of effects from none to total cladding failure. I don't claim the parameters in the input file have any particular meaning. If we want to use this model, its there, but we have to come up with acceptable input parameters.

8. The schoepite model makes the assumption that all radionuclides are captured by the schoepite and only released at the rate the schoepite dissolves. This is unrealistically optimistic for I-129 and Tc-99, but more reasonable for Np-237. The basis is explained in the papers Bill Murphy and I wrote. The schoepite model assumes that the schoepite dissolves, but this rate is very slow compared with the release rates for models 1 and 2. Surface area will have little effect, as explained above, since its the solubility limit of the schoepite that affects the rate.

I would be happy to discuss these tests with you, and could do the further runs if I had your test conditions.

Dick

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From: Richard Codell

Created By: Richard.Codell@nrc.gov

Recipients:
"Andy Campbell" <Andy.Campbell@nrc.gov>
Tracking Status: None
"David Esh" <David.Esh@nrc.gov>
Tracking Status: None
"Timothy McCartin" <Timothy.McCartin@nrc.gov>
Tracking Status: None
"Ronald Janetzke" <rjanetzke@cnwra.swri.edu>
Tracking Status: None
"Sitakanta Mohanty" <smohanty@cnwra.swri.edu>
Tracking Status: None

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