November 10, 1994

Dr. Prasad K. Nair, Manager
CNWRA EBS Program Element
CNWRA/San Antonio Office
Southwest Research Institute
6220 Culebra Road
San Antonio, TX 78238-5166

SUBJECT: EBS PROGRAM ELEMENT INTERMEDIATE MILESTONE NO. 20-5702-523-510, EBS Performance Assessment Codes (EBSPAC) Progress Report, as transmitted on October 28, 1994.

Reference: 1. "Engineered Barrier System Performance Assessment Codes (EBSPAC) Progress Report October 1, 1993, through September 25, 1994," CNWRA No. 94-026, October 1994.

2. Operations Plans for the Division of Waste Management for FY94-95 (Ops Plans), EBS Section 3.5.1.4, Subtask 2.3, (Revision 4, change 3): Investigation of Issues Related to the EBS.

Dear Dr. Nair:

The report of Reference 1 has been reviewed and the staff finds that it fulfills the requirements of subject deliverable, which is called for under the FY94-95 Operations Plans, Reference 2. Comments by EBS staff members, T. Ahn and D. Dancer, are enclosed for your consideration in future work.

If you have any questions regarding this matter, please contact me at (301) 415-6652.

Sincerely,

Charles G. Interrante
EBS Program Element Manager
Engineering and Geosciences Branch
Division of Waste Management
Office of Nuclear Safety
and Safeguards

Enclosure: As stated

cc: J. Linehan, PMDA
B. Meehan, DCPM

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COMMENTS ON REPORT NO. CNWRA 94-026, "ENGINEERED BARRIER SYSTEM PERFORMANCE ASSEMENT CODES (EBSPAC) PROGRESS REPORT, OCTOBER 1, 1993, THROUGH SEPTEMBER 25, 1994 - David Dancer & Tae Ahn

1. Because of the numerous equations and symbols used within the report, there should be a separate Nomenclature section.

2. In Section 2.0, the description of the CTOUGH Code is inadequate. Specifically, CNWRA should discuss (or cite the reference for) the following:

   - the Nonsymmetric Preconditioned Conjugate Gradient (NSPCG) package
   - the Nested factorization algorithm
   - the D4 direct solver
   - the Evaporation Rate Computation algorithm
   - the Relative Humidity Computation algorithm

3. In Section 3.2, there should also be a comparison of the code GEM with the crevice corrosion code developed by Watson (Watson, 1989 and Watson and Postlethwaite, 1990).

4. In section 3.2, the report discusses the changes that GEM makes to the TWITCH/MARIANA codes. Omitted from this section was any discussion of the flux calculation scheme. Therefore, we presume that the flux calculation scheme will continue to be the hybrid scheme described in the previous progress report (Sridhar et. al., 1993). The latter scheme uses a first-order upwind method for high Peclet numbers. It should be noted that the American Society of Mechanical Engineering's Journal of Fluids Engineering (Freitas, 1993), acting on the advice of the Coordinating Group on Computational Fluid Dynamics, has recently banned the use of first-order upwind methods in papers submitted for publication. The AIAA Journal (AIAA, 1994) and the International Journal for Numerical Methods in Fluids (Gresho and Taylor, 1994) have recently adopted policies that, while not explicitly banning the use of first-order upwind methods, will make the use of such methods extremely onerous. The rationale for these actions are succintly described by Roache (Roache, 1994a):

   > The reasons for the blanket rejection of first-order methods were well stated, succintly and accurately, by Freitas in the cited editorial, and are well recognized by all honest CFD practictioner. The issue has become something of a joke, and the joke is getting stale. ("The good news about first-order upstream differencing is that it always gives you an answer. The bad news is that it always gives you the same answer, no matter what the Reynolds number.") . . . the analysis of the artificial viscoscity effect of first-order upstream differencing has been well known for over a quarter of a century! Experience and devastating comparisons fill the literature."

Enclosure

CNWRA's use of first-order numerical techniques (see also Comments 6 and 9), coupled with CNWRA's failure to conduct the usual grid refinement studies (e.g., Roache, 1994b) impair the credibility of EBSPAC.

5. On the last line of page 3-5, what does " electron does not occur" mean?

6. In Section 3.6, there should be an explanation of why CNWRA chose the fully implicit integration scheme. The latter algorithm has only first- order temporal accuracy and is usually not recommended (Greenspan, 1978, Ferziger, 1981, Ames, 1977, and Carnahan et. al., 1969). More logical choices would appear to be the Crank-Nicholson method (Greenspan, 1978, Ferziger, 1981, Ames, 1977, Carnahan et. al., 1969, Carslaw and Jaeger, 1959, Crank, 1975, and Roache, 1972), the method of lines coupled with higher order backward implicit methods (Gear, 1971 and Oran and Boris, 1987), or the method of lines coupled with Lawrence Livermore Laboratory's ODEPACK (Hindmarsh, 1987). It should be noted that CNWRA used a variation of ODEPACK in the SCCEX code (Cragnoli et. al., 1994 and Torng et. al., 1994). CNWRA should also describe the time step strategy that they employed. It is well known (Prothero, 1976) that implicit schemes are generally not useful in solving transient problems unless the time step is changed in the course of the computation.

7. For the results given in Sections 4, 5, and 6, it is essential that CNWRA provide information on the temporal and spatial discretizations used. This is particularly important given the first-order time integration scheme, first-order upwind convective scheme, and first-order boundary treatment that CNWRA used (see Comments 4, 6, and 9).

8. In section 7, it is not clear why once the conditions for stress corrosion cracking were established, crack initiation was assumed to occur after an induction period of 20 years.

9. Notwithstanding CNWRA's assertion to the contrary, CNWRA did not use the fictitous point method in the derivations in Section B.2. Using the fictitious point method, Equations B-28 and B-30 should be:

$$\Psi_{j,N+1} = \Psi_{j,N-1} \qquad \text{(B-28a)}$$

$$\Psi_{j,-1} = \Psi_{j,1} \qquad \text{(B-30a)}$$

Similarly, Equations B-29 and B-31 need to be revised. It should be noted that the scheme used by CNWRA is only first-order accurate and is usually not recommended (Carslaw and Jaeger, 1959 and Crank, 1975). In the classical study by Price and Slack (Price and Slack, 1952), CNWRA's scheme was found to perform poorly compared to the fictitious point method and other methods considered.

10. On page B-3, equation B-13 is incorrect (There should be a coefficient of 2 on the right hand side).

11. On page B-3, equation B-15 is incorrect (the term p^2 should be replaced with the partial derivative symbol ∂).

12. On pages B-11 and B-12, the derivation of equations B-69 through B-75 is not obvious. It appears that those equations are inconsistent with equations B-44 through B-46.

13. This progress report extended the previous version of EBSPAC. For instance, a thermodynamic data base has been installed in the code. However, the users may need to know more about the following:

- The author indicates that all reactions were described in a more general way. Then, benchmark examples were given. We consider that the generalization may have been rather a posteriori constructed from benchmark examples. We would like clarification, as we are not sure of the meaning of generalization, as used in the report. What is its advantage over separate, simple descriptions of each problem area or discipline? If the generalization means more than this, some applications should be made, using the generalization. How is the generalization applied to chemical problems, especially in HLW? In many chemical problems, we generally know what should be described once we know the governing physical processes and a generalization is not needed for physical proceses.

- The report addresses the progress made to save computation time in light of the long period of times over which repository behavior must be estimated. Is this a real problem? A problem may not even exist if dimensions are properly converted. For instance, diffusivity in cm^2/second can be converted to m^2/1000 years to be compatible with the dimensions used in evaluations of the system performance. Irrespective of the time scale, we consider (as did the author) that the real problem is the stability of iteration errors.

- The advantage of using the asymptotic solution has been addressed. As considered in the above comment, the importance (or unimportance) of transient phenomena depends on the interval. A short mathematical transient time can sometimes be very long in reality. Additionally, problems that require initiation times (e.g., localized corrosion) may require either an actual estimate or data that is made by other (non-asymptotic) means.

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