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6/21/89

Dr. Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6431
Sandia National Laboratories
P. O. Box 5800
Albuquerque, NM 87185

Dear Dr. Cranwell:

Please find enclosed a set of review comments for the draft document (NUREG/CR-4766) entitled "User's Manual for the NEFTRAN Computer Code." Also attached is a separate set of comments from Richard Codell of the Hydrology Section. Contact me at FTS 427-4131 if you have any questions about the enclosures.

The action taken by this letter is considered to be within the scope of the current contract A1158. No changes to cost or delivery of contracted services and products are authorized. Please notify me immediately if you believe that this letter would result in changes to cost or delivery of contracted products for project A1158.

Sincerely,

(Original Signed by

Neil M. Coleman, Project Manager
Hydrology Section
Technical Review Branch
Division of High-Level Waste Management

Enclosures:
As stated

cc: C. Harlan, Sandia
P. Davis, Sandia

Wm-RES
WM Record File
A1158
SWL

WM Project 10,11,16
Docket No.
PDR ✓
LPDR ✓ (B, N, S)

Distribution:

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WM Project: WM-10,11,16
PDR w/encl
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REVIEW COMMENTS
NEFTRAN USER'S MANUAL

1. For all computer programs, and particularly for a code such as NEFTRAN that is designed to be computationally efficient, knowledge of simplifying assumptions and limitations of the code are important to the user. These assumptions and limitations are indeed discussed in the text. However, it would prove especially useful for new user's of NEFTRAN to provide a more concise summary of this information. Therefore, it is recommended that the code capabilities, simplifying assumptions and limitations be summarized in a chart at the end of Chapter 2.

2. It is noted that the discussion of chemical inputs to the code is fairly limited. Because the chemical input is a K_d (or retardation factor), the use of which can be somewhat controversial, a discussion of the K_d approach may be needed. Most studies involving retardation effects depend on the application of distribution coefficients (K_d). These coefficients are based on and derived from idealized chemical reactions, with the result that in actual use an investigator may over- or under-estimate the retardation factor for a particular medium. Accordingly, it is recommended that some discussion be provided to guide the user in how to select proper K_d values and how to properly interpret model results based on them. If appropriate and readily available literature exists that would provide this information, then it may be sufficient to introduce this topic along with a set of relevant references.

Editorial Comments

page 5, last para., lines 1 and 2: for both lines, change "c f." to "cf."

page 8, para. 2, line 10: change "depository" to "repository"

page 24, para. 2, line 4: change "identify" to "identity"

page 39, para. 1, last sentence: please clarify whether the "difference" discussed in this sentence is an improvement or merely a difference between the code versions

page 41, para. 1, line 2: remove the hyphen from the expression "two-points"

page 42, last equation: this equation may be in error - please confirm its validity

page 96, para. 1, line 8, 1st word: replace "The" with "These"

page 97, line 5: change "convection" to "convention"

page 105, para. 2, line 5: delete the extra comma that follows the word "by"

COMMENTS ON NEFTRAN USERS MANUAL
BY Richard Codell

I am generally impressed with the manual. It is full of information on the derivation and limitations of the methods. The code will be the mainstay of our efforts to assess performance of at least the saturated repository sites and perhaps the unsaturated site (NNWSI) as well. There is sufficient information in the manual for an involved person to set up, run and understand the input and results.

One comment I would like to make concerns the form of the source term model for the mixing cell approach. I feel that this is a useful model, but that future development of the code should include a boundary layer diffusion model which accounts for the buildup of dissolved radionuclides close to the canisters. Such an approach was developed by Kerrisk, et al. at Los Alamos. The concepts are not difficult to understand and appear in standard textbooks on mass transfer as well. The idea behind such a mass transfer model is that releases from the canister are limited in some cases by the buildup of concentration close to the canister, especially for those radionuclides which have a high rate of release from the uranium oxide matrix. This phenomenon is not taken into account in the mixing cell model, and may overestimate the rate of release in some cases. While this is conservative, the boundary layer model is simple and defensible. I have talked about this approach informally with Sandia personnel in the past, but the task has not been proposed formally. I think that it would be a valuable addition to the method.

Another comment I have about the manual is that I was unable to look at the computer code. I hope that you intend to include the code listing in the manual, at least in microfiche form. Inspection of the code is important for a thorough review. Since this is an update of an old computer code, I wanted to examine whether good programming practices were followed or if this was simply a patch job on the old code, a la SWIFT. It would be highly preferable for the code to follow state-of-the-art programming practices such as structured programming according to the F77 standard. Such procedures are essential to improve the quality assurance of software.

I think that the extensive computer outputs in the back of the manual should be relegated to microfiche format in order to reduce the length of the text.

There are several references to an improved model for matrix diffusion to replace the present two-compartment model. I think that this would be a valuable addition to NEFTRAN. I was under the impression that the money for this task has been approved and that there was no longer any question about the replacement. If so, the text of the manual on pages 44 and 116 should reflect this.

I question the general validity of the statement on page 8, middle of page that "..a thermal model has not been included since thermal effects from the radioactive waste are confined to a relatively small region about the

depository." A number of scaling and model studies have amply demonstrated that thermally induced buoyant pressures can sometimes be a major factor in determining the flow magnitude and direction, and that such effects can last for many thousands of years. In fact, the thermal effects can be incorporated by defining the pressures in a different model such as SWIFT as input to NEFTRAN. The statement on the thermal effects is inaccurate and should be modified to allow for the possibility of significant thermal effects.