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Albuquerque, New Mexico 87185

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July 15, 1986

Mr. John Peshel
Engineering Branch
Division of Waste Management
U.S. Nuclear Regulatory Commission
7915 Eastern Avenue
Silver Spring, MD 20910

Dear Mr. Peshel:

The enclosed monthly report summarizes the activities during the month of June for FIN A-1755.

If you have any questions, please feel free to contact me at FTS 844-8368 or E. J. Bonano at FTS 844-5303.

Sincerely,

Robert M. Cranwell
Supervisor
Waste Management Systems
Division 6431

RMC:6431

Enclosure

Copy to:
Office of the Director, NMSS
Attn: Program Support Branch
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PROGRAM:	Coupled Thermal-Hydrological-Mechanical Assessments and Site Characterization Activities for Geologic Repositories	FIN#:	A-1755
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD:	10/85 - 9/86
DRA PROGRAM MANAGER:	J. Peshel	BUDGET AMOUNT:	226K
CONTRACT PROGRAM MANAGER:	R. M. Cranwell	FTS PHONE:	844-8368
PRINCIPAL INVESTIGATORS:	E. J. Bonano	FTS PHONE:	844-5303
	L. R. Shipers	FTS PHONE:	846-3051

PROJECT OBJECTIVES

To provide technical assistance to NRC in the assessment of coupled thermal-hydrological-mechanical phenomena and site characterization activities for high-level waste repositories.

ACTIVITIES DURING JUNE 1986

Activities and Accomplishments

During the month of June the previously reported current month and year-to-date expenditures were examined. As indicated in previous monthly reports, the year-to-date expenditures are not accurate. The discrepancies have been identified and procedures are now in progress to correct them. An explanation of the actions taken to correct these discrepancies is included.

The review of one of the BWIP documents sent by John Buckley has been completed and is included as an attachment to this report.

Travel

None.

Problems Encountered

None.

DOE/INTERNATIONAL
PERFORMANCE ASSESSMENT
DOCUMENT REVIEW

AUTHOR: Rockwell Hanford Operations

TITLE: EPASTAT: A Computer Code for Estimating Radionuclide Releases at the Accessible Environment Boundary from a Repository in Basalt

REFERENCE INFORMATION: SD-BWI-TA-022, REV 0; January 1986

DOCUMENT
SUMMARY: The EPASTAT computer code was developed as a part of the Basalt Waste Isolation Project (BWIP) to obtain an estimate of the cumulative radionuclide release reaching the accessible environment in a specified time after the closure of a high-level nuclear waste repository in basalt. The code was designed as a link of results from waste-package-scale, repository-scale, and regional-scale models in an effort to assess the overall long term performance of the repository. The code is based upon the simplifying assumption that the overall system behavior is both linear and lumped, so that all heterogeneities and time dependent behavior have been neglected. This code is stochastic in nature and is intended to be used for parametric and sensitivity analysis studies. Since this computer code is based upon a deterministic model with random input variables, it is possible to perform a fully deterministic analysis with this code by specifying all of the input variables as constants.

The radionuclide transport is analyzed using a simple one-dimensional flow tube model that includes the effects of water velocity, retardation, and dispersion/diffusion. An option to neglect the dispersive effect in the transport model does exist within the code. The flux released from the waste packages must be specified as a boundary condition for the transport model. This data may be either read from a file (in a format consistent with the output of another BWIP code) or calculated internally by the EPASTAT code. Both solubility limited release and leach limited release models are included as options for the internal calculation of the source flux term. The ground-water travel time, one of the controlling parameters for transport, must be specified as an input to the EPASTAT computer code. The effective transport porosity, adsorption (distribution) coefficient, as well as other problem specific parameters and material properties must also be given as input data. The primary model output consists of a table of values of the cumulative radioactive flux crossing a hypothetical boundary located at a given distance along the flow tube. These cumulative flux values are reported as a ratio with respect to the EPA limits set for radionuclide release. The time at which a

nonzero concentration of a radionuclide reaches the specified boundary may also be reported. A users manual for the EPASTAT computer code is included as an appendix of the report.

DESCRIPTION OF MATHEMATICAL MODELS: For one-dimensional transport along the main flow direction of a radionuclide in a homogeneous medium, the governing equation is

$$n R_D \frac{\partial C}{\partial t} + u' \frac{\partial C}{\partial x} = n D' \frac{\partial^2 C}{\partial x^2} - \lambda n R_D C \tag{1}$$

where

n = effective porosity (dimensionless)

R_D = retardation coefficient (dimensionless)

C = $C(x,t)$ = concentration at distance x and time t (curies per liter)

t = time (years)

u' = Darcy velocity (meters per year)

x = distance from the source along the streamline (meters)

D' = dispersion coefficient (meters squared per year)

λ = radioactive decay constant (one per year)

The initial and boundary conditions are

$$C(x,0) = 0 \quad \text{for } x>0 \tag{2a}$$

$$-D' n \frac{\partial C}{\partial x} + u' C \Big|_{x=0} = q(t) \tag{2b}$$

$$C(\infty,t) = 0 \text{ for } t \geq 0 \tag{2c}$$

where $q(t)$ is the source flux term. When the concentration is expressed as a product of an appropriately chosen exponential function and an initially unknown function of time and location, Eq. (1) may be transformed to the standard form of the one-dimensional, transient diffusion equation. The analytical solution to this transformed partial differential equation and its appropriately transformed initial and boundary conditions is available. This solution, expressed in terms of the original variables, is

$$C(x,t) = \frac{2}{nR_D\sqrt{\pi D}} \int_0^\infty \exp\left(\frac{-uw}{2D}\right)$$

$$\int_{\frac{x+w}{2\sqrt{Dt}}}^{\infty} \exp\left[\frac{ux}{2D} - \left(\frac{u^2}{4D}+\lambda\right)\frac{(x+w)^2}{4Dz^2} - z^2\right] q\left(t - \frac{(x+w)^2}{4Dz^2}\right) dz\,dw \qquad (3)$$

where $D = D'/R_D$ and $u = u'/(nR_D)$. From this expression, the flux at any location x and time t may be determined using the relationship

$$q(x,t) = -D'\, n \frac{\partial C}{\partial x} + u'\, C \qquad (4)$$

The cumulative flux may then be evaluated by integrating Eq. (4) over the time period of interest.

When the dispersive effects are neglected (D'= 0 in Eqs. (1) and (2b)), the resulting governing differential equation may be solved by the Laplace transformation method. Using this method, a closed form analytical solution results for the concentration when the flux source term, q(t), is assumed to be piecewise linear in form. When this concentration solution is used to evaluate the instantaneous flux and this flux is, in turn, integrated with respect to time, the cumulative flux can be shown to be

$$Q(x,t) = \exp(-\lambda x/u) \Bigg\{ \sum_{k=1}^{n} [(t^2_{k+1} - t^2_k + 2x(t_{k+1}-t_k)/u)a_k/2$$

$$+ (b_k - (t_k + x/u)a_k)(t_{k+1}-t_k)] + (t^2 - (t_j + x/u)^2)a_j/2$$

$$+ (b_j - (t_j + x/u)a_j)(t - (t_j + x/u)) \Bigg\} \qquad (5)$$

where b_k is the value of q(t) at time t_k, a_k is the slope of the function q(t) between times t_k and t_{k+1}, and j is the index such that $t_j\ t<t_{j+1}$.

When the source flux term is internally calculated, it is assumed that all of the containers in the repository fail simultaneously. Also, neither of the source flux models used can deal with the case of the inventory of a daughter radionuclide increasing with time due to the decay of a parent nuclide. When the solubility limited release model for the calculation of the source flux term is used, it is assumed that when release begins that the saturation limit is instantly attained and that this saturation concentration is maintained until the inventory is depleted. This results in a rectangular pulse release for the source flux.

Two simplifying assumptions are embedded in the leach limited release model: first, that the glass matrix leaches at a constant rate for a finite number of years and second, that the amount of radionuclide contained in the portion of the matrix that leaches is immediately dissolved in the ground-water and becomes available for transport. An exponential term is also included in the source flux term in order to account for radionuclide decay.

NUMERICAL IMPLEMENTATION: As can be seen from Eq. (3), it is necessary to evaluate a double integral to determine the concentration, and thus the flux, at a given point in time and space when dispersion is included in the model. To determine the cumulative flux another integration must be performed, resulting in the evaluation of a triple integral. These integrations were performed numerically using a combination of Gauss-Legendre and Laguerre procedures. It should be noted that when dispersion effects are neglected that this numerical integration is not performed because a closed form solution, Eq. (5), is available. In all cases, the flux source term, q(t), was assumed to be piecewise linear. The decision of whether or not to include dispersion effects is based upon the value of the Peclet number. The Peclet number was defined as ux_A/D where x_A is the distance to the accessible environment. At high Peclet numbers the dispersion effect in the transport was considered negligible. Also, precision problems were encountered in the evaluation of the integrals of the general model at high Peclet numbers. Based on a distance of 5 km to the accessible environment, when the Peclet number was greater than 4000 dispersion effects were neglected. An option does exist within the code to force the more general dispersion model to be used, but for high Peclet numbers the accuracy of the results is in doubt.

The parameters in the general transport model that are treated as random variables are the effective dispersion coefficient, effective transport porosity, retardation coefficient, and Darcy velocity. Of these variables only the effective transport porosity is directly sampled. The remaining three quantities are calculated from other sampled variables. The additional parameters that are used in these calculations that may be treated as random variables are the adsoption coefficient, travel time, molecular diffusion coefficient, and dispersivity. If the flux source term is internally calculated by the code, several additional parameters may be specified as random variables. In the solubility limited release model the water flow rate may be treated as a random variable. When the leach limited release is specified, the leach duration may be treated as a random variable. In both cases, time of the failure of the containers may be specified as a random variable. Uniform, normal, lognormal, loguniform, and exponential distributions may be specified for sampling of the stochastic variables. If desired, these distributions may be truncated between some user specified limits. An option for a user supplied probability distribution also exists within the code. A Monte Carlo sampling technique is used to generate the input vectors for the random variables.

LIMITATIONS: The EPASTAT computer code was designed to be a stand alone FORTRAN program with options and feature which are machine independent. This is not true of the plot features of the code which use the proprietory DISPLA graphics system (obtained under contract from Integrated Software Systems Corporation) and are tailored for interactive use with a Tektronix 4054 graphics terminal. When dispersion is included in the model interactive use of the code is not recommended due to large run times. In order to provide graphics support for the code in the batch environment, an option to write data to a file for postprocessing is included in the code. To analyze this data an additional code, EPAPLT, which is not documented in the report is necessary. While the input data files for a sample problem and the resulting code output are included in the Users Manual, no comparison of the results with another analytical or numerical solution was performed. As stated on the cover page, the EPASTAT computer code has not been validated and benchmarked for use in licensing of a repository.

The computer code is based upon a simple, lumped parameter, one-dimensional transport model. The effects of transport through layers with different properties and the travel times within these layers cannot be directly modelled. It should be noted that from the references cited for ground-water travel times it is not clear that travel times based upon single media calculations will be used in the model. There is also an apparent inconsistency in the procedure for specifying input data for the code. Travel time is required as an input to the code. The calculation of travel time requires the use of an effective porosity. Yet in the EPASTAT computer code the travel time and the effective porosity are sampled independently of one another. This results in calculations using the effective porosity, retardation factors, Darcy velocities, etc., not being consistent with those used to evaluate travel times. Also, the basic assumption that flow in basalt, a fractured media, can be modelled as flow in a homogeneous media must be questioned.

OTHER COMMENTS: An error exists in Eq. (A-12) on page 24, as this is not the Laplace transform of Eq. (A-10). Also in the paragraph preceeding Eq. (A-12) on page 24 the notation used for the concentration and its transform is not consistent.

Reviewed by: L. R. Shipers, June 1986

A-1755
1628.010
June 1986

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

		Current Month	Year -to- Date
I.	Direct Manpower (man-months of charged effort)	0.6	7.7
II.	Direct Loaded Labor Costs	5.0	79.0
	Materials and Services	0.0	0.0
	ADP Support (computer)	0.0	6.0
	Subcontracts	8.0	212.0
	Travel	0.0	1.0
	Other (computer roundoff)	0.0	1.0
	TOTAL COSTS	13.0	299.0*

III. Funding Status

Prior FY Carryover	FY 86 Projected Funding Level	FY 86 Funds Received to Date	FY 86 Funding Balance Needed
31K	226K	195K	None

*A credit of $60,000 in SAIC charges is being assessed to the project. These additional charges resulted from the payment of an SAIC invoice during the period following Krishan Wahi's departure from SAIC and the close-out of the SAIC contract on A-1755.

Additional credits totalling about $20,000 are also being assessed to this project resulting from erroneous charges from Remote Sensing (an SNLA contractor) and Jack Daeman. The charges for Jack Daeman are due to SNLA's procedure of "accuring" funds in anticipation of charges from a contractor. Since Jack Daeman has not worked on this project this year, the accured funds will be credited to A-1755.

These credits should appear on the next monthly budget report. Additional credits may also appear on subsequent monthly budget reports.