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SOFTWARE RELEASE NOTICE

01. SRN Number: GHGC-SRN-163

02. Project Title: Performed for SDMP Project Work | Project No.: 10-8001-004

03. SRN Title: NEFTRAN II, LLW Version 1.0

04. Originator/Requestor: Randy Pedors | Date: 12.10.97

05. Summary of Actions

- ☒ Release of new software
- ☐ Release of modified software:
  - ☐ Enhancements made
  - ☐ Corrections made
- ☐ Change of access software
- ☒ Software Retirement

12/13/2001

06. Persons Authorized Access

Name	RO/RW	A/C/P
Rand Pedors	RW	A
Amit Armstrong	RO	A
Ralph Cady (NRC)	RO	A
Dick Codell (NRC)	RO	A
Pat LaPlante	RO	A
Tims McCartin (NRC)	RO	A
Mark Thaggard (NRC)	RO	A
Jim Winsrle	RO	A
Gordon Wittmeyer	RO	A

07. Element Manager Approval: Date: 12/23/97

08. Remarks:

(CNWRA Form TYP-6 09/00)

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SOFTWARE SUMMARY FORM

01. Summary Date: 12.01.97	02. Summary prepared by (Name and phone) Randy Fedors 210.522.6818		03. Summary Action: New
04. Software Date: 11.19.97	05. Short Title: NEFTRAN II, LLW V. 1.0		
06. Software Title: NEFTRAN II; Low Level Waste Version 1.0			07. Internal Software ID: N/A
08. Software Type: ☐ Automated Data System ■ Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ■ Batch ☐ Combination	10. Application Area A. General: ■ Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other B. Specific:	
11. Submitting Organization and Address: CNWRA/SWRI 6220 Culebra Road San Antonio TX 78228		12. Technical Contact(s) and Phone: Tim McCarin 301.415.6681	
13. Narrative: Network model for groundwater flow and radionuclide transport with source term which includes dissolution, diffusion, and rinse.			
14. Computer Platform: PC	15. Computer Operating System:DOS or Windows	16. Programming Language(s): Fortran 77	17. Number of Source Program Statements: 9456
18. Computer Memory Requirements: 4 MB	19. Tape Drives: N/A	20. Disk/DrumUnits: > 10MB	21. Graphics: N/A
22. Other Operational Requirements: None			
23. Software Availability: ■ Available ☐ Limited ☐ In-House ONLY		24. Documentation Availability: ■ Available ☐ Inadequate ☐ In-House ONLY	
Software Custodian: [signature] Date: 12/19/97			

CNWRA Form TOP-4-1

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES 3/29

SOFTWARE CONTROL CHECKLIST

Name of Software: NEFTRAN II **Version:** Low Level Waste VERSION 1.0

Primary User: Randy Fedors

☐	SOFTWARE REQUIREMENTS DESCRIPTION	
	Documentation	☐
☐	DESIGN AND DEVELOPMENT	
	Documentation	N/A
☐	DESIGN VERIFICATION	
	Computer runs uniquely identified	N/A
	Software analysis tools have been applied and discrepancies resolved	N/A
	Design Verification Report	☐
X	INSTALLATION TESTING	
	Installation test documentation	X
	Discrepancy resolution	☐
X	CONFIGURATION CONTROL	
	Software Summary Form	X
	User's Manual and data files.	X
	Technical Description	X
	Source Code	X
	Version Control - **Version number created**	X
	Software Release Notice	X
☐	SOFTWARE PROBLEM REPORTING AND RESOLUTION	
	Software Problem and Change Request	☐
☐	SOFTWARE VALIDATION	
	Software Validation Test Plan	☐
	Software Validation Test Report	☐
☐	SOFTWARE RETIREMENT	
	Software Release Notice	☐

NEFTRAN II, Low Level Waste Versior ' 0 Software

4/29

To Mail List:#SA-WO TECH STAFF
To: Amit Armstrong at CNWRA-SUN
To: Charles Connor at CNWRA
To: Randall Fedors at CNWRA-SUN
To: David Ferrill at CNWRA
To: Amitava Ghosh at CNWRA-SUN
To: Ronald Green at CNWRA-SUN
To: Simon Hsiung at CNWRA-SUN
To: Ronald Janetzke at CNWRA-SUN
To: Mark Jarzemba at CNWRA
To: Peter Lichtner at CNWRA-SUN
To: Ronald Martin at CNWRA-SUN
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To: John Stamatakos at CNWRA
To: Stuart Stothoff at CNWRA-SUN
To: James Weldy at CNWRA-SUN
To: Jim Winterle at CNWRA-SUN
To: Gordon Wittmeyer at CNWRA-SUN
cc: MEhnstrom@swri.edu at Internet
cc: Maria Padilla
bcc: Bruce Mabrito
From: Bruce Mabrito
Subject: NEFTRAN II, Low Level Waste Version 1.0 Software
12-22-1997 08:32 PM

The Low Level Waste version of NEFTRAN II software has been put under configuration (version) control in accordance with TOP-018 requirements. A version of 1.0 was assigned to this "NEFTRAN II LLW software" to clearly differentiate it from the TPA module of NEFTRAN, per B. Sagar's request. The TPA NEFTRAN module is "TOP-018-controlled" under the TPA "umbrella."

The Software Release Notice has been signed by John Russell and the primary users have been identified as R. Fedors, A. Armstrong, P. LaPlante, J. Winterle, G. Wittmeyer, T. McCartin (NRC), M. Thaggard (NRC), R. Cady (NRC), R. Codell (NRC).

The CNWRA Master Directory of Scientific and Engineering Software will be updated and distributed to CNWRA technical staff next week.

If you have questions re control of NEFTRAN II LLW Version 1.0, contact me; if you have technical question re NEFTRAN II LLW Version 1.0, contact Randy Fedors or Tim McCartin. Bruce Mabrito

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

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TWINBROOK METRO PLAZA, #210
12300 TWINBROOK PARKWAY
ROCKVILLE, MD 20852-1606

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TO: Bruce Mabrito

COMPANY: CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

FROM: JOHN RUSSELL

COMPANY: CNWRA — WASHINGTON OFFICE

TELEPHONE: (301) 881-0289

MESSAGE: Bruce,

Transmitted is NEFTRAN II, LLW Version 1.0 Software Release Notice with my signature for EM approval.

John

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NEFTRAN II

As of today (12-19-97) the source code give to me on diskette for Neftran II has been placed under SCCS control. Below are the specifics.

Program Name:	Neftran II
Date Entered:	19 Dec 1997
Control Method:	SCCS
Version Number:	1.0
Location:	mammoth:/lan/rcs/neftran_llw_1.0
Code Type:	Fortran

I have provided a list of the files and a diskette with the exact files that were placed under control.

Ray Kotara
Technical Specialist I

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```
total 694
drwxr-xr-x   2 root     other        512 Dec 19 11:39 .
drwxr-xr-x  46 root     other       1536 Dec 19 11:30 ..
-rwxrwxrwx   1 root     other      55741 Jan 25  1995 diflch.rec
-rwxrwxrwx   1 root     other      28389 Oct  2 18:04 dvm1.tjm
-rwxrwxrwx   1 root     other      48158 Oct  2 18:05 dvm2.tjm
-rwxrwxrwx   1 root     other      16945 May  8  1997 flow.for
-rwxrwxrwx   1 root     other        462 Nov 19 13:58 nefiitjm.for
-rwxrwxrwx   1 root     other      40599 Dec 16 13:25 nefmain.for
-rwxrwxrwx   1 root     other       1478 Dec 19 11:40 readme
-rwxrwxrwx   1 root     other       3938 Jul 31 15:02 readsrc.for
-rwxrwxrwx   1 root     other       9586 Nov 18 13:49 setdis.for
-rwxrwxrwx   1 root     other        532 Nov  3 11:55 sizes.inc
-rwxrwxrwx   1 root     other      46282 Jul 31 15:19 source.for
-rwxrwxrwx   1 root     other      32161 Feb  8  1993 stopper.for
-rwxrwxrwx   1 root     other      30692 Apr 14  1994 work.for
-rwxrwxrwx   1 root     other      30442 Sep 17 15:55 xport.for
```

NAMES and sizes of
Files on NEFTRAN II LLW Version 1.0

Dennis Mahoney 12/19/97

8/29

TO: Bruce Mabrito
FROM: R. Fedors
SUBJECT: TOP-018 for NEFTRAN II Low Level Waste Version 1.0
DATE: December 16, 1997

The NEFTRAN II code is written and documented by Sandia National Laboratory (NUREG/CR-5618). A modified version has been incorporated into the Total-System Performance Assessment (TPA) code (version 3.1.1, September 26, 1997) for the high level waste program. The NEFTRAN II module is under TOP-018 control as part of the TPA code performance assessment work. Another version, the standalone program, contains all of the same modifications as the module in the TPA code according to Tim McCartin (per. comm. Nov. 20, 1997) of NRC. A portion of the NEFTRAN II documentation (NUREG/CR-5618) is included in the TOP-018 file for the Low Level Waste (LLW) version; interested users are referred to the TOP-018 folder and the SPCRs for the TPA code for documentation of the modifications made prior to November 20, 1997. The LLW version contains one additional modification not included in the NEFTRAN II TPA module, an enhanced source term module.

The addition of a more sophisticated leach module is primarily for low-level waste work by NRC researchers. This leach module was adapted by Tim McCartin from the BLT code written and documented by Terry Sullivan at Brookhaven National Laboratory (NUREG/CR-5387). Tim McCartin has forwarded to us a copy of the letter to Mark Thaggard (NRC) from Terry Sullivan which states that McCartin's leach module for NEFTRAN II correctly implements the leach portion of BLT as documented in NUREG/CR-5387. A portion of the BLT documentation as well as the letter from T. Sullivan are included in the TOP-018 folder for the LLW version of NEFTRAN II.

There was no version number associated with the LLW version of NEFTRAN II as received from NRC. A version number is required for CNWRA TOP-018 control, hence the name of the program and the source code have been modified to reflect version number control. It will now be referred to as NEFTRAN II Low Level Waste Version 1.0 dated December 16, 1997. Since the original NEFTRAN II from Sandia National Laboratory as well as the changes to the code noted above are adequately documented, it was determined that only an installation test was required prior to TOP-018 release of the program. The only modification to the source code as received from NRC (Nov 20, 1997) is: (I) comment lines at the top of the nefmain.for file indicating the version number; and, (ii) format statement 70 in the flowin subroutine contained in the nefmain.for file was changed such that the version number will be printed at the top of the output file.

Part of decision on which code will be used for low level waste work such as the Site Decommissioning Management Plan (SDMP) lies in the capabilities of the new leach module. These may be a desirable attribute to add additional flexibility for SDMP leaching work. The leach module increases the flexibility for modeling the leach rate. The original NEFTRAN II uses a solubility-based model with either linear or exponential approaches. The solubility of each radionuclide controls the transfer from source mass to water leaving the source mass area. The linear model uses a fraction of the original mass while the exponential model accounts for a decreasing source mass of radionuclides by taking a fraction of the remaining amount. The new leach module approximates three different processes; solubility, diffusion, and dissolution models. Diffusion rate and dissolution rate appropriate for each radionuclide are inputs for the leach module. Solubilities are a part of the original NEFTRAN II. Fractions of each process are input parameters with the total of the solubility, diffusion, and dissolution fractions summing to one. In addition, parameters for container life, container degradation rate, and container diffusion rate are additional inputs which may constrain the leach rate from the source mass.

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The implementation of the leach module within the NEFTRAN II code is handled in a similar fashion to other modules. Depending on the value of an input flag, the leach input file is read and the leach module is executed. The flag can also be used to specify that the original NEFTRAN II leach rate calculation be performed. The flag switch is in line 17 of the main input file and is commented as "EXTERNAL SOURCE FLAG (=1 use TJM Subroutine; >1 read UNIT 14." Input instructions for the leach module are incorporated as comments in the code; a sample printout of the input file is include in the TOP-018 folder. It should be noted that the same radionuclides must be included in the leach input file as were input in the main NEFTRAN II input file.

The code is compiled on a personal computer running Win95 using the Lahey Fortran 77 compiler. The program code is organized as separate files. The executable is created by compiling and linking the file "nefiitjm.for" which contains the separate files as include statements. The executable "nefiitjm.exe" was added to the floppy diskette which contains the source code. After typing the executable name at the DOS prompt, the user will be prompted for the main input file name. Other input files should use the same root name; e.g., randy.inp (main input file), randy.tjm (new source term input), randy.vel (velocity field data). Lahey Fortran 90 did not compile this code due to variable type problems with some of the intrinsic function calls. In addition, the code will not compile on UNIX machines unless the PC-based functions are modified.

The installation test uses input files created by Tim McCartin. Three input files are required for NEFTRAN II if the special leach module is to be used; the two standard input files plus an input file with information specific to the leach rate options. The input files are included on the diskette for the TOP-018 file. The output of the installation test (rwf.out) is included on the floppy diskette which contains the code. The UNIX command "diff" was run on McCartin's output file (randy.out) and my output file (rwf.out) with the result indicating that the only difference was the time stamp and the addition of a version number at the top of the output file. Thus a proper installation of the LLW version of the NEFTRAN II code was made on personal computers running DOS or Windows.

Attachments:
Floppy diskette with source code, sample input files, and executable file
Software Summary Report (draft)
Software Release Notice (draft)
Software Summary Form (draft)
Excerpts from NUREG/CR-5618, User's Manual for the NEFTRAN II Computer Code
Excerpts from NUREG/CR-5387, Low-Level Waste Shallow Land Disposal Source Term-Model: Data Input Guides
Letter from Sullivan to Thaggard, correct implementation of BLT source term
Sample input file for leach module

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How to enter Source into SCCS

1. Create directory under /lan/rcs on Mammoth.

2. Copy all files into created directory.

3. Execute "sccs enter *" while in the directory.

4. This will create a SCCS sub-dir with all the files under control.

5. You may now delete all the files in the created directory starting with a ",".

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NUREG/CR–5618
SAND90–2089

User's Manual for the NEFTRAN II Computer Code

Prepared by
N. E. Olague, D. E. Longsine, J. E. Campbell, C. D. Leigh

Sandia National Laboratories
Operated by
Sandia Corporation

Prepared for
U.S. Nuclear Regulatory Commission

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NUREG/CR-5618
SAND90-2089
RW

User's Manual for the NEFTRAN II Computer Code

Manuscript Completed: January 1991
Date Published: February 1991

Prepared by
N. E. Olague, D. E. Longsine[1], J. E. Campbell, C. D. Leigh

Sandia National Laboratories
Albuquerque, NM 87185

Prepared for
Division of Engineering
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555
NRC FIN A1266

[1]Intera, Inc., Austin, TX

ABSTRACT

This document describes the NEFTRAN II (NEtwork Flow and TRANsport in Time-Dependent Velocity Fields) computer code and is intended to provide the reader with sufficient information to use the code. NEFTRAN II was developed as part of a performance assessment methodology for storage of high-level nuclear waste in unsaturated, welded tuff. NEFTRAN II is a successor to the NEFTRAN and NWFT/DVM computer codes and contains several new capabilities. These capabilities include: 1) the ability to input pore velocities directly to the transport model and bypass the network fluid flow model, 2) the ability to transport radionuclides in time-dependent velocity fields, 3) the ability to account for the effect of time-dependent saturation changes on the retardation factor, and 4) the ability to account for time-dependent flow rates through the source regime. In addition to these changes, the input to NEFTRAN II has been modified to be more convenient for the user. This document is divided into four main sections consisting of 1) a description of all the models contained in the code, 2) a description of the program and subprograms in the code, 3) a data input guide and 4) verification and sample problems. Although NEFTRAN II is the fourth generation code, this document is a complete description of the code and reference to past user's manuals should not be necessary.

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LOW-LEVEL WASTE SHALLOW LAND DISPOSAL SOURCE TERM-MODEL: DATA INPUT GUIDES

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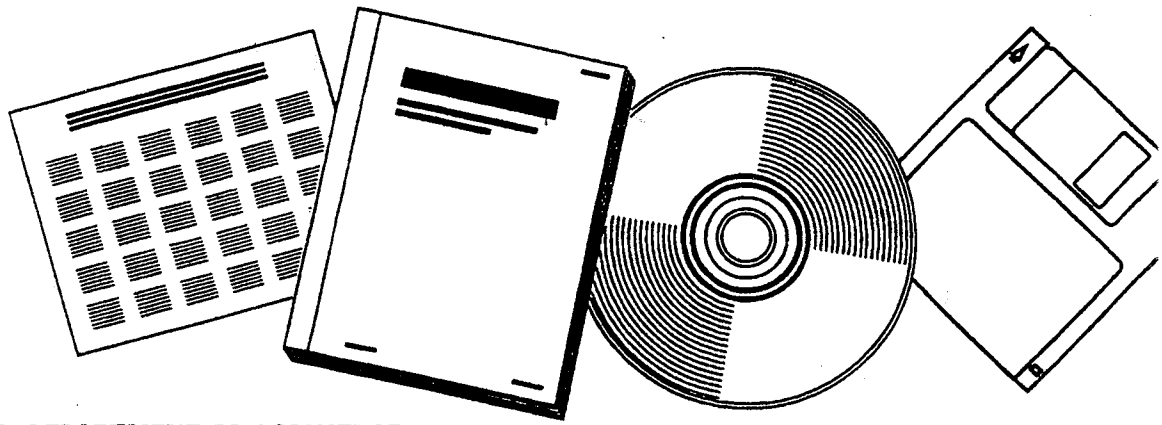
BROOKHAVEN NATIONAL LABORATORY
UPTON, NY

JUL 89



U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

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NRC FORM 335 (8-87) NRCM 1102, 3201, 3202

U.S. NUCLEAR REGULATORY COMMISSION

BIBLIOGRAPHIC DATA SHEET

SEE INSTRUCTIONS ON THE REVERSE

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NUREG/CR-5387
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Low-Level Waste Shallow Land Disposal Source Term Model: Data Input Guides

4. DATE REPORT COMPLETED

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May	1989

5. AUTHOR(S)

T. M. Sullivan, C. J. Suen

6. DATE REPORT ISSUED

MONTH	YEAR
July	1989

7. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code)

Brookhaven National Laboratory
Upton, NY 11973

8. PROJECT/TASK/WORK UNIT NUMBER

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Division of Engineering
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555

11a. TYPE OF REPORT

FORMAL

b. PERIOD COVERED (Inclusive dates)

12 SUPPLEMENTARY NOTES

13. ABSTRACT (200 words or less)

This report provides an input guide for the computational models developed to predict the rate of radionuclide release from shallow land disposal of low-level waste. Release of contaminants depends on four processes: water flow, container degradation, waste from leaching, and contaminant transport. The computer code FEMWATER has been selected to predict the movement of water in an unsaturated porous media. The computer code BLT (Breach, Leach, and Transport), a modification of FEMWASTE, has been selected to predict the processes of container degradation (Breach), contaminant release from the waste form (Leach), and contaminant migration (Transport). In conjunction, these two codes have the capability to account for the effects of disposal geometry, unsaturated/saturated water flow, container degradation, waste form leaching, and migration of contaminants released within a single disposal trench. In addition to the input requirements, this report presents the fundamental equations and relationships used to model the four different processes previously discussed. Further, the appendices provide a representative sample of data required by the different models.

14. DOCUMENT ANALYSIS - a. KEYWORDS/DESCRIPTORS

Low-Level waste
Source Term modeling
Unsaturated water flow
Metallic container degradation
Waste form leaching
Unsaturated Contaminant Transport

b. IDENTIFIERS/OPEN-ENDED TERMS

15. AVAILABILITY STATEMENT

Unlimited

16. SECURITY CLASSIFICATION

(This page) Unclassified

(This report) Unclassified

17. NUMBER OF PAGES

327

18. PRICE

NUREG/CR-5387
BNL-NUREG-52206
RW

Low-Level Waste Shallow Land Disposal Source Term Model: Data Input Guides

Manuscript Completed: May 1989
Date Published: July 1989

Prepared by
T. M. Sullivan, C. J. Suen

Brookhaven National Laboratory
Upton, NY 11973

Prepared for
Division of Engineering
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
NRC FIN A3276

ABSTRACT

This report provides an input guide for the computational models developed to predict the rate of radionuclide release from shallow land disposal of low-level waste. Release of contaminants depends on four processes: water flow, container degradation, waste from leaching, and contaminant transport. The computer code FEMWATER has been selected to predict the movement of water in an unsaturated porous media. The computer code BLT (Breach, Leach, and Transport), a modification of FEMWASTE, has been selected to predict the processes of container degradation (Breach), contaminant release from the waste form (Leach), and contaminant migration (Transport). In conjunction, these two codes have the capability to account for the effects of disposal geometry, unsaturated/saturated water flow, container degradation, waste form leaching, and migration of contaminants released within a single disposal trench. In addition to the input requirements, this report presents the fundamental equations and relationships used to model the four different processes previously discussed. Further, the appendices provide a representative sample of data required by the different models.

EXECUTIVE SUMMARY

The objective of the source term evaluation project is to provide a system model capable of predicting radionuclide release rates from a low-level radioactive waste shallow land burial trench. The first topical report for this project [Sullivan, 1987] presented the framework for developing the system model. The problem was separated into four compartments: water flow, container degradation, waste form leaching, and radionuclide transport. This compartmental approach provides the flexibility to easily incorporate model improvements and new models. The second topical report [Sullivan et al., 1988] discussed the models used to represent each of the four compartments. After thorough review, the computer code FEMWATER and FEMWASTE were chosen to represent the processes of unsaturated groundwater flow and contaminant transport, respectively. Models were developed to predict container corrosion and waste form leaching. Each of these models was individually tested. Since that time, FEMWASTE has been modified to include the models for container degradation, and leaching. The resulting code is named BLT, (Breach, Leach, and Transport).

This report presents the necessary information required for using the computer codes FEMWATER and BLT. This includes: the theory and basic equations for the four different processes; the step by step procedure to be followed when running the codes; input guides, and examples of data required by the models.

FEMWATER is a two-dimensional finite element code capable of predicting water velocity, moisture content, and pressure head in an unsaturated/saturated porous media. The theory and equations along with limitations of FEMWATER are discussed in Chapter 2.

BLT is a two-dimensional finite element code capable of predicting container degradation, waste form leaching, and radionuclide migration in an unsaturated porous media. The container degradation subroutine models pitting and general corrosion processes of metallic containers. The leaching model considers three independent release mechanisms: solubility limited release due to surface wash-off (the rinse model), solubility limited release due to dissolution of the waste form, and diffusion controlled release. The amount of material released from the waste form also depends on the amount of container area that has been breached by corrosion. The transport model considers advection, dispersion, diffusion, and chemical retardation. Radioactive decay is considered in the leaching and transport compartments. The theory and equations along with limitations of BLT are presented in Chapter 3.

In general, each of these four processes ar interdependent. In practice, groundwater flow is assumed to be independent of the other three processes. However, the remaining three compartments, (namely, container degradation, waste form leaching, and radionuclide transport) all depend on results from the groundwater flow calculation (moisture content and velocity). Waste form leaching also depends on the fraction of the container that has been breached due to corrosion, and also on solubility effects. The input to the transport equation is the amount released from the waste form. The exact procedure to couple all of these processes is described in Chapter 4.

Chapters 5 - 8 provide the detailed information necessary to use FEMWATER and BLT. Chapter 5 presents the procedure for setting up an input deck for FEMWATER. Chapter 6 discusses the types of problems that can be solved using FEMWATER and BLT and presents some examples. Chapter 6 also includes a sample input deck for FEMWATER. Chapter 7 is the data input guide for FEMWATER. It presents all of the information required to create an input deck for the code. An example of the main (printer) output file from FEMWATER is in Appendix 14. Chapter 8 is the data input guide for BLT. It consists of three segments, the data guide, an annotated inut file, and an annotated main output file. In FEMWATER and BLT specifying the finite element mesh, boundary conditions, and initial conditions can be tedious. Both codes incorporate special input formats that help minimize repetitive input. Examples of how to use these features are provided in the input guides.

There are 15 appendices to this report. These appendices provide representative data for the various models and additional information useful in running the codes.

In principle, each of the models requires site-specific data. To facilitate the use of the codes, representative data have been compiled from the literature and are provided in the appendices. These include data for soil properties in the unsaturated zone, metallic corrosion, cement waste form leaching, solubility limits in soil systems, retardation factors, dispersion coefficients in the unsaturated zone, and expected radionuclide inventories. For the inventories, the potential of ingrowth of radionuclide daughters from transuranic nuclides has been evaluated.

Additional information has been provided to help understand the special features in FEMWATER and BLT. For example, the relationship between hydraulic conductivity and permeability, relationships between mass and volume, initial conditions, and application of boundary conditions, are explored in further detail in the appendices. To further illustrate the use of special input features, appendices discussing automatic finite element mesh numbering and variable array dimensioning procedure are also provided.

Special features of BLT discussed in the appendices are: (1) the output files which can be used for graphics applications; (2) redimensioning the finite element grid to reduce problem size; (3) restart capabilities which allow a problem to be restarted as the calculation proceeds (this allows rate properties such as water flow rate, corrosion rate, transport properties, etc., to undergo step changes as a function of time); (4) the program structure.

CONTENTS

CONTENTS (continued)

DF 7/8/97

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BROOKHAVEN NATIONAL LABORATORY
ASSOCIATED UNIVERSITIES, INC.

P.O. Box 5000
Upton, New York 11973-5000
TEL (516) 282-2840
FAX (516) 282-5305
E-MAIL

Department of Advanced Technology

September 30, 1993

Mr. Mark Thaggard
U.S. Nuclear Regulatory Commission
NMSS/LLWB
Mail Stop 5-E4 Room 5-F19
Washington, DC 20555

Dear Mark:

I have reviewed the modifications to NEFTRAN made by Dr. Tim McCartin to incorporate the BLT wasteform leaching models for rinse, diffusion and dissolution into NEFTRAN. In general, the changes were extremely well documented within the code and easy to follow. The review included a line by line comparison of the coded release equations to those found in the BLT manual. The release rates are calculated correctly.

I also reviewed the coupling between the release models and the NEFTRAN model. In the absence of solubility constraints, the releases feed directly into the transport equation used in NEFTRAN, and this is done correctly. Although the NEFTRAN method for preventing releases to cause the concentration to exceed the solubility limit differs from that found in BLT, the NEFTRAN approach is valid and properly implemented.

In conclusion, the release models found in the subroutine DIFLCH of the NEFTRAN code are consistent with those found in BLT.

Sincerely,

Terry

Terry Sullivan, Group Leader
Performance and Risk Assessment

TS:al

```
0.000E+00 : Dissolutional-release container lifetime (yr)
1.000E+02 : Rinse-release container lifetime (yr)
5.000E+01 : Diffusional-release begin time (yr)
7.300E+00 : Diffusional-release container volume (cf)
1.000E+00 : Diffusional-release container radius (ft)
1.000E+02 : Diffusional-release Degradation
1.000E+02 : Degraded Diffusion begin time (yr)
DECAY-CHAINS ARRAYS FOR VARIABLE WASTE-FORM LEACHING:
```

Name A6	Fraction for Rinse#1	Diffusion Rate (ft**2/year)	Fraction for diff.	Dissolution Rate (ft/year)	Fraction for dis.	Dis. Radius (feet)
'CM246'	0.800E+00	3.000E-07	0.200E+00	6.200E-04	0.000E+00	5.000E-02
'U238 '	0.800E+00	3.000E-07	0.200E+00	6.200E-04	0.000E+00	5.000E-02
'CM245'	0.800E+00	3.000E-07	0.200E+00	6.200E-04	0.000E+00	5.000E-02
'AM241'	0.800E+00	3.000E-07	0.200E+00	6.200E-04	0.000E+00	5.000E-02
'NP237'	0.800E+00	3.000E-07	0.200E+00	6.200E-04	0.000E+00	5.000E-02
'AM243'	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'PU239'	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'PU240'	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'U234 '	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'TH230'	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'RA226'	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'PB210'	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'CS135'	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'I129 '	0.000E+00	3.000E-07	1.000E+00	6.200E-04	0.000E+00	5.000E-02
'TC99 '	0.000E+00	3.000E-07	0.000E+00	6.200E-04	1.000E+00	5.000E-02
'NI59 '	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'C14 '	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'SE79 '	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'NB94 '	1.000E+00	3.000E-07	0.000E+00	6.200E-04	0.000E+00	5.000E-02
'CL36 '	0.000E+00	3.000E-07	1.000E+00	6.200E-04	0.000E+00	5.000E-02

Sample Input file for leach module

26/29

```
c******************< File NefMain.FOR; April 28, 1997 >************************
cZDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD?
c3 Modified by R. Cady to run under the Lahey F77L-EM/32 FORTRAN compiler.     3
c3   The modifications consist of:                                            3
c3       1. Adding GETDAT and GETTIM subroutines that mimic the Microsoft     3
c3          routines.                                                         3
c3       2. Adjusting the FORM in OPEN statements for UNFORMATTED files       3
c3          rather than BINARY files.                                         3
c3       3. Inserting some commas within format statements where required.     3
c3       4. Adjusting the code to use the explicit GETCL routine from         3
c3          Lahey to get the command-line argument that is intended to        3
c3          supply the input filename.                                        3
c3       5. Revising the RATIO subroutine to reflect the previous (non-PC)    3
c3          version logic.  The code in the PC version did not execute        3
c3          properly! {Properly as defined by the mainframe version.}         3
c3       6. Revise a format statements to print chain numbers with two        3
c3          digits rather than sometimes only a single digit.                 3
c3       7. Revise the total number of chains allowed.  In the present        3
c3          version this was set at six by the number of files dimensioned    3
c3          by FN.  Also set the starting file number for scratch files to 51 3
c3       8. Modify vector dimensions in subroutine SRCIN to * rather than 1   3
c3          to allow Lahey bounds-checking on enumerated dimensioned arrays.  3
c3          Also in SRCIN, correct dimension of S() to MXISO.                 3
c3       9. Modify SOURCE and LECHMOD subroutines to allow the leaching of    3
c3          isotopes at isotope-specific rates by making FLCH a vector.       3
c3          Also modify SOURCE subroutine to zero out an inventory only       3
c3          if both the source rate AND number of atoms are less than one.    3
c3      10. Modify FLOWIN to call an independent input routine for TJM's      3
c3          addition of BLT-like source term.                                 3
c3      11. Modify COMMON ISOTOP to place LAMBDA first for proper alignment   3
c3          since LAMBDA is double precision.                                 3
c3      12. Modify SOURCE and main to allow source rates (CI/YR) to be        3
c3          input from an external file as described by TJ McCartin's         3
c3          note to Budhi Sagar dated February 18, 1992.                      3
c3      13. Modify WORK to allow interpolation of discharges in the event     3
c3          that truncation of incremented time causes end-of-file while      3
c3          reading chain discharges.  Sets final discharge to last input.    3
c3      14. Modify DTUPDT to call DTDIFLCH if DIFLCH is active to determine   3
c3          a maximum timestep to capture the diffusion and dissolution peaks.3
c3      15. Modify WORK to incorporate information on step velocity changes   3
c3          in the interpolation of discharges to a common basis.  This       3
c3          interpolation now does not interpolate across a step change and   3
c3          simply maintains the previous discharge up to the step and then   3
c3          uses the subsequent discharge after the step change.              3
c3      16. Modify SOURCE to adjust the source flux in the event of time      3
c3          varying velocity.  Prior implementation followed the time series  3
c3          of velocity BUT source flux was linearly interpolated while       3
c3          velocity is sequential steady steps.  So force source flux to     3
c3          change stepwise also if velocity is time varying.                 3
c3      17. Modify TRNSPT to calculate the source flux via SRCIN to be        3
c3          consistent by determining the source for the first half of the    3
c3          time step and the last half of any preceding time step.           3
c3      18. Modify WORK to allow a value of IOPT(13) > 1 to force the output  3
c3          of discharge in {ROOT}.Dis to retain the isotope peaks even if    3
c3          they occur within a tenth of a time step from another output time.3
c3      19. Modify WORK to allow an I6 format for the number of discharge     3
c3          steps within an individual isotope time series.  Previous format  3
c3          was I4.                                                           3
c3      20. Modify WORK to allow a value of IOPT(13) < -1 to filter the       3
c3          discharge output to {ROOT}.Dis to retain only the essential       3
c3          information; delete segments of time series that remain constant. 3
c3      21. Insert pause statements prior to STOP within DVM1.FOR & DMV2.FOR  3
c3          to allow user to view errors at the point that they occur.        3
c3      22. In subroutine ADJB within DVM2.FOR, statement labeled 150 starts  3
c3          an infinite loop if IC > 1.  I suspect that this loop should be   3
c3          repeated only DSMX/DX(LG) times; not infinitly.                   3
```

```
c3       23. In DXDT, revise DXK to be dimensioned by MXPTH rather than by     3
c3           MXMEM!  It turns out that it is used that it does not really      3
c3           need to be dimensioned but is addressed by migration path.        3
c@DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDY
      PROGRAM NEF
C
C   ************************************************************************
C   *              ISSUED BY SANDIA NATIONAL LABORATORIES (SNL)             *
C   *                      A PRIME CONTRACTOR TO THE              *
C   *                  UNITED STATES DEPARTMENT OF ENERGY                    *
C   *                          *
C   *  THIS COMPUTER CODE WAS PREPARED UNDER WORK SPONSORED BY THE UNITED    *
C   *  STATES GOVERNMENT.  NEITHER THE UNITED STATES, NOR THE UNITED STATES  *
C   *  DEPARTMENT OF ENERGY, NOR ANY OF THEIR EMPLOYEES, NOR ANY OF THEIR    *
C   *  CONTRACTORS, SUBCONTRACTORS, OR THEIR EMPLOYEES, MAKE ANY WARRANTY,   *
C   *  EXPRESS OR IMPLIED, OR ASSUME ANY LEGAL LIABILITY OR RESPONSIBILITY   *
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C   *  WOULD NOT INFRINGE PRIVATELY OWNED RIGHTS.                            *
C   *                          *
C   ************************************************************************
C   *                          *
C   *    CODE NAME       -  NEFTRAN II (NETWORK FLOW AND/OR   *
C   *              TRANSPORT WITH TIME-DEPENDENT     *
C   *              VELOCITIES)                       *
C   *                          *
C   *    VERSION     -  PC MICROSOFT FORTRAN VERSION      *
C   *              RELEASED OCTOBER 1990             *
C   *                          *
C   *    DESCRIPTION        -  THIS CODE IS AN ENHANCED VERSION  *
C   *              OF THE NEFTRAN (NETWORK FLOW AND  *
C   *              TRANSPORT) CODE DOCUMENTED IN     *
C   *              NUREG/CR-4766.  NEFTRAN II        *
C   *              SIMULATES SATURATED GROUND-WATER  *
C   *              FLOW WITH A NETWORK FLOW MODEL.   *
C   *              NEFTRAN II SIMULATES GROUND-WATER *
C   *              RADIONUCLIDE TRANSPORT USING THE  *
C   *              DISTRIBUTED VELOCITY METHOD (DVM).*
C   *              TRANSPORT CAN BE COUPLED WITH THE *
C   *              RESULTS OF THE NETWORK FLOW MODEL *
C   *              OR FROM GROUND-WATER VELOCITIES   *
C   *              SUPPLIED BY THE USER.  THESE      *
C   *              VELOCITIES CAN BE TIME-DEPENDENT  *
C   *              IN THE FORM OF SEQUENTIAL STEADY- *
C   *              STATE VELOCITIES.  THIS IS THE    *
C   *              ENHANCED CAPABILITY OF NEFTRAN II *
C   *              COMPARED TO NEFTRAN.  NEFTRAN II  *
C   *              ALLOWS FOR THE TRANSPORT OF       *
C   *              MULTIPLE CHAINS OF ANY LENGTH,    *
C   *              WITH ISOTOPES HAVING DIFFERENT    *
C   *              RETARDATIONS, AND WITH SOURCE     *
C   *              RATES BEING LEACH- AND/OR         *
C   *              SOLUBILITY-LIMITED.  NEFTRAN II   *
C   *              ALSO PROVIDES THE CAPABILITY TO   *
C   *              MODEL THE SOURCE AS A MIXING CELL *
C   *                      AND TO MODEL MATRIX DIFFUSION.    *
C   *                          *
C   *    PURPOSE     -  NEFTRAN II WAS DEVELOPED AS PART  *
C   *              OF A PERFORMANCE ASSESSMENT       *
C   *              METHODOLOGY FOR A HIGH-LEVEL      *
C   *              RADIOACTIVE WASTE REPOSITORY      *
C   *              LOCATED IN UNSATRATED, FRACTURED  *
C   *              MEDIA.        *
C   *                          *
C   *    LANGUAGE    -  ANSI STANDARD FORTRAN, VERSION77  *
C   *                          *
```

```
C  *     HARDWARE    -  PC (MEMORY REQUIREMENT DEPENDS     *
C  *                 ON SIZE OF PROBLEM)                 *
C  *                          *
C  *     COMPILER    -  MICROSOFT FORTRAN VERSION 5.0      *
C  *                          *
C  *     LIBRARIES        -  NONE                  *
C  *                          *
C  *     PREDECESSORS        -  THE NETWORK FLOW AND TRANSPORT     *
C  *                 (NWFT) MODEL, SNL, 1978-1979       *
C  *                 NWFT/DVM MODEL, SNL, 1979-1981     *
C  *                 GENNET, SNL, 1984            *
C  *                 NEFTRAN, SNL, 1987           *
C  *                          *
C  *     DOCUMENTATION       -  (1)  NWFT/DVM USER'S MANUAL          *
C  *                NUREG/CR-2081, SAND81-0886    *
C  *                  (2)  NWFT/DVM VERIFICATION         *
C  *                NUREG/CR-3378, SAND83-1466    *
C  *                  (3)  NEFTRAN USER'S MANUAL         *
C  *                NUREG/CR-4766, SAND86-2405    *
C  *                  (4)  NEFTRAN II USER'S MANUAL      *
C  *                NUREG/CR-5618, SAND90-2089    *
C  *                (ALL INCLUSIVE)              *
C  *                          *
C  *     SANDIA CONTACTS     -  NATALIE E. OLAGUE        *
C  *                  PHILIP I. POHL               *
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C  *                          *
C  ********************************************************************************
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