


1/29

SOFTWARE RELEASE NOTICE

01. SRN Number: GHQC-SRN-163																																
02. Project Title: Performed for SDMP Project Work		Project No.: 10-5001-004																														
03. SRN Title: NEPTRAN H, LLW Version 1.0																																
04. Originator/Requestor: Randy Peders		Date: 12.10.97																														
05. Summary of Actions <ul style="list-style-type: none"> <input checked="" type="checkbox"/> Release of new software <input type="checkbox"/> Release of modified software: <ul style="list-style-type: none"> <input type="checkbox"/> Enhancements made <input type="checkbox"/> Corrections made <input type="checkbox"/> Change of access software <input checked="" type="checkbox"/> Software Retirement 																																
06. Persons Authorized Access <table border="1"> <thead> <tr> <th>Name</th> <th>RO/RW</th> <th>A/C/D</th> </tr> </thead> <tbody> <tr><td>Rand Peders</td><td>RW</td><td>A</td></tr> <tr><td>Arak Armstrong</td><td>RO</td><td>A</td></tr> <tr><td>Ralph Cady (NRC)</td><td>RO</td><td>A</td></tr> <tr><td>Dick Codell (NRC)</td><td>RO</td><td>A</td></tr> <tr><td>Pat LaPlante</td><td>RO</td><td>A</td></tr> <tr><td>Time McCartin (NRC)</td><td>RO</td><td>A</td></tr> <tr><td>Mark Thaggard (NRC)</td><td>RO</td><td>A</td></tr> <tr><td>Ira Winters</td><td>RO</td><td>A</td></tr> <tr><td>Gordon Wittmeyer</td><td>RO</td><td>A</td></tr> </tbody> </table>			Name	RO/RW	A/C/D	Rand Peders	RW	A	Arak Armstrong	RO	A	Ralph Cady (NRC)	RO	A	Dick Codell (NRC)	RO	A	Pat LaPlante	RO	A	Time McCartin (NRC)	RO	A	Mark Thaggard (NRC)	RO	A	Ira Winters	RO	A	Gordon Wittmeyer	RO	A
Name	RO/RW	A/C/D																														
Rand Peders	RW	A																														
Arak Armstrong	RO	A																														
Ralph Cady (NRC)	RO	A																														
Dick Codell (NRC)	RO	A																														
Pat LaPlante	RO	A																														
Time McCartin (NRC)	RO	A																														
Mark Thaggard (NRC)	RO	A																														
Ira Winters	RO	A																														
Gordon Wittmeyer	RO	A																														
07. Element Manager Approval: <i>[Signature]</i>		Date: 12/23/97																														
08. Remarks:																																

2/29

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: <input type="checkbox"/> Automated Data System <input checked="" type="checkbox"/> Computer Program <input type="checkbox"/> Subroutine/Module	09. Processing Mode: <input type="checkbox"/> Interactive <input checked="" type="checkbox"/> Batch <input type="checkbox"/> Combination	10. Application Area A. General: <input checked="" type="checkbox"/> Scientific/Engineering <input type="checkbox"/> Auxiliary Analyses <input type="checkbox"/> Total System PA <input type="checkbox"/> Subsystem PA <input type="checkbox"/> 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/Drum Units: > 10MB	21. Graphics: N/A
22. Other Operational Requirements: None			
23. Software Availability: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Limited <input type="checkbox"/> In-House ONLY		24. Documentation Availability: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Inadequate <input type="checkbox"/> In-House ONLY	
Software Custodian: 		Date: 12/19/97	

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

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

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 Hslung 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
To: Sitakanta Mohanty at CNWRA
To: William Murphy at CNWRA
To: Goodluck Ofoegbu at CNWRA-SUN
To: David Pickett at CNWRA
To: James Prikryl at CNWRA
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**

5/29

**TWINBROOK METRO PLAZA, #210
12300 TWINBROOK PARKWAY
ROCKVILLE, MD 20852-1606****FAX/TELECOPIER NO: (301) 881-0294****FAX (TELECOPY) COVER SHEET****DATE:**12/22/97**NO. OF PAGES
(INCLUDING COVER PAGE)**2**FAX/TELECOPIER NO.
CALLED:**(210) 522-~~6081~~**IF ALL PAGES NOT
RECEIVED, CALL**

(301) 881-0289 BARBARA LONG or Speed No. 298

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 NEFTPAW II, LLW
Version 1.0 Software Release Notice
with my signature for EM
approval.

John

RECEIVED

DEC 22 1997

CNWRA

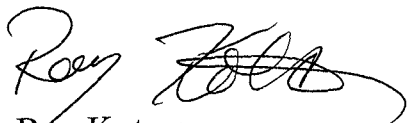
6/29

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

7/29

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 NEPTRAN II LLW Version 1.0

Samuel S. S. 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.

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

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 ",".

11/29

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

407.24 --- T199303090012
User's Manual for the NEFTRAN
II Computer
Code-NUREG/CR-5618
SAND90-2089

User's Manual for the NEFTRAN II Computer Code

Manuscript Completed: January 1991
Date Published: February 1991

Prepared by
N. E. Olague, D. E. Longsine¹, 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

¹Intera, Inc., Austin, TX

RECEIVED
MAR 12 1991
CNWRA-WO

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.

14/29

TABLE OF CONTENTS

	<u>Page</u>
1.0 INTRODUCTION	1-1
1.1 Background	1-1
1.2 Purpose	1-1
1.3 Report Structure	1-3
2.0 DESCRIPTION OF MODELS	2-1
2.1 Network Flow Model	2-2
2.1.1 Theory	2-2
2.1.2 Implementation	2-3
2.1.3 Fluid Density and Viscosity Submodels	2-5
2.2 Analytical Transport Model	2-7
2.2.1 Theory	2-8
2.2.2 Implementation	2-8
2.3 Source Model	2-12
2.3.1 Theory	2-13
2.3.2 Implementation	2-18
2.4 Distributed Velocity Method (DVM) Transport Model	2-21
2.4.1 Theory	2-21
2.4.2 Implementation	2-25
2.4.3 Time Step Determination	2-33
2.4.4 Spatial-Step Determination	2-35
2.4.5 Courant Numbers and Isotope Travel Times	2-36
2.4.6 Species Velocity Model	2-47
2.4.7 Discharge Model	2-49
2.4.8 Distribution of Source Into Grid Blocks	2-49
2.4.9 Leg-to-Leg Transfer Model	2-50
2.4.10 Matrix Diffusion Model.....	2-54
2.4.11 DVM Transport in Time-Dependent Velocity Fields	2-59
3.0 DESCRIPTION OF CODE	3-1
3.1 Structure	3-1
3.1.1 General	3-1
3.1.2 Source Module	3-3
3.1.3 Transport Module	3-3

15/29

TABLE OF CONTENTS

	<u>Page</u>
3.2 Subroutines	3-3
3.2.1 NEFMAIN - main program	3-6
3.2.2 ADJB(VA, LG, IP, TS, ILAST, KNT)	3-6
3.2.3 BAND(TSTART, TEND)	3-6
3.2.4 BRANCH(EPS)	3-7
3.2.5 BSOLVE(KER)	3-7
3.2.6 CATCH(GA, NPT, VDT)	3-7
3.2.7 CHAIN(IW)	3-7
3.2.8 CHKPTH	3-8
3.2.9 COEFF	3-8
3.2.10 DTUPDT	3-8
3.2.11 DXDT	3-8
3.2.12 ET	3-9
3.2.13 FACER	3-9
3.2.14 FLOWIN(IPASS, ROOT, KROOT)	3-9
3.2.15 GETRV(JTRIAL)	3-10
3.2.16 GIT(T, Y, V, AL)	3-10
3.2.17 INPRIN(MM, INCRM)	3-10
3.2.18 INTG(S1,B1,S2,B2,T1,T2,D,F,N,DT,ANS)	3-10
3.2.19 LECHMOD(T1,T2,F)	3-11
3.2.20 METHOD	3-11
3.2.21 MXCLL(KBMAX)	3-11
3.2.22 PRP(D,B,V,VP,DL,N,T1,T2)	3-11
3.2.23 PTHLEN	3-12
3.2.24 RATIO(DJ,DI,TIME,RAT)	3-12
3.2.25 SETDIS	3-12
3.2.26 SETUP	3-13
3.2.27 SIFT(NSORT, TSCL)	3-14
3.2.28 SOURCE(IPASS, JTRIAL)	3-14
3.2.29 SRCIN(T,SR1,SR2,TS1,TS2,N1,N2,NTOTX,S24,IEOF)	3-15
3.2.30 STOPPER(ISTOP)	3-16
3.2.31 TIMER(KNT)	3-16
3.2.32 TPPRT(TM, TSET)	3-16
3.2.33 TRACER(K, TT, PDIS)	3-17
3.2.34 TRNSPT(T, TSET, NTP, NPT, KALL)	3-17
3.2.35 TSPFAC(DT, D, B, LT, TDP)	3-18
3.2.36 WORK(IPASS, JTRIAL)	3-18
3.2.37 XCHNG	3-19
3.3 Parameter Statements	3-19
3.4 Common Blocks	3-20
4.0 DATA INPUT GUIDE	4-1
4.1 Execution Procedure for NEFTRAN II	4-1
4.2 General Input Description	4-2
4.3 Parameter Input Description	4-3
4.3.1 Options	4-3
4.3.2 Problem Size Parameters	4-10

16
29

TABLE OF CONTENTS

	<u>Page</u>
4.3.3 Source and Flow Parameters	4-12
4.3.4 Time Parameters	4-14
4.3.5 Increment-Determination Parameters	4-15
4.4 Array Input Description	4-19
4.4.1 Network Leg Properties Array	4-20
4.4.2 Junction Properties Array	4-21
4.4.3 Migration Path Properties Array	4-22
4.4.4 Decay Chain Array	4-24
4.4.5 Element Properties Array	4-27
4.5 Data Required for Multiple Simulations	4-29
4.5.1 Multiple Data Sets	4-29
4.5.2 Use of Subroutine GETRV	4-31
4.6 Sample Input File.....	4-31
5.0 VERIFICATION AND SAMPLE PROBLEMS	5-1
5.1 Sample Problem 1 - DVM and Analytical Transport Model.....	5-1
5.1.1 Reference Site	5-1
5.1.2 Network Flow Model	5-5
5.1.3. Data Set #1	5-5
5.1.4 Data Set #2	5-19
5.1.5 Results	5-20
5.2 Sample Problem 2 - Matrix Diffusion	5-20
5.3 Sample Problem 3 - Time-dependent DVM Velocities	5-29
6.0 REFERENCES.....	6-1
APPENDIX A Species Velocity Model.....	A-1
APPENDIX B Discharge Model.....	B-1
APPENDIX C Distribution of Source Into Migration Path Using Mixing-Cell Model.....	C-1
APPENDIX D Storage of Decay Chain Information.....	D-1
APPENDIX E Output Files for Sample Problems.....	E-1



NUREG/CR-5387

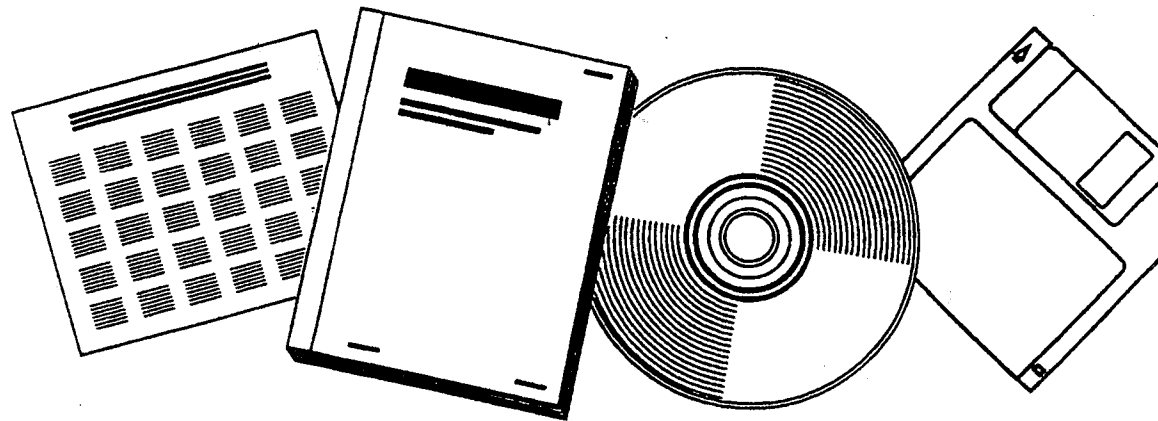
NTIS
Information is our business.

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

17/
29


BROOKHAVEN NATIONAL LABORATORY
UPTON, NY

JUL 89



U.S. DEPARTMENT OF COMMERCE
Information Service

350
--- T199708060002
Low-Level Waste Shallow Land
Disposal Source Term Model:
Data Input Guides

<small>NRC FORM 336 (8-87) NRCM 1102, 3201, 3202</small>		<small>U.S. NUCLEAR REGULATORY COMMISSION</small>		<small>18/29</small> <small>ORT NUMBER (Assigned by PPMB: DPS, add Vol. No., if any)</small>					
BIBLIOGRAPHIC DATA SHEET			NUREG/CR-5387 BNL-NUREG-52206						
<small>2. TITLE AND SUBTITLE</small> Low-Level Waste Shallow Land Disposal Source Term Model: Data Input Guides			NUREG/CR-5387 						
<small>5. AUTHOR(S)</small> T. M. Sullivan, C. J. Suen			<small>4. DATE REPORT COMPLETED</small> <table style="width: 100%; border: none;"> <tr> <td style="width: 50%; text-align: center;"><small>MONTH</small></td> <td style="width: 50%; text-align: center;"><small>YEAR</small></td> </tr> <tr> <td style="text-align: center;">May</td> <td style="text-align: center;">1989</td> </tr> </table>			<small>MONTH</small>	<small>YEAR</small>	May	1989
<small>MONTH</small>	<small>YEAR</small>								
May	1989								
<small>7. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code)</small> Brookhaven National Laboratory Upton, NY 11973			<small>6. DATE REPORT ISSUED</small> <table style="width: 100%; border: none;"> <tr> <td style="width: 50%; text-align: center;"><small>MONTH</small></td> <td style="width: 50%; text-align: center;"><small>YEAR</small></td> </tr> <tr> <td style="text-align: center;">July</td> <td style="text-align: center;">1989</td> </tr> </table>			<small>MONTH</small>	<small>YEAR</small>	July	1989
<small>MONTH</small>	<small>YEAR</small>								
July	1989								
<small>10. SPONSORING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code)</small> Division of Engineering Office of Nuclear Regulatory Research U.S. Nuclear Regulatory Commission Washington, DC 20555			<small>8. PROJECT/TASK/WORK UNIT NUMBER</small> <small>9. FIN OR GRANT NUMBER</small> FIN A-3276						
<small>12. SUPPLEMENTARY NOTES</small>			<small>11a. TYPE OF REPORT</small> FORMAL <small>b. PERIOD COVERED (Inclusive dates)</small>						
<small>13. ABSTRACT (200 words or less)</small> <p>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.</p>									
<small>14. DOCUMENT ANALYSIS - a. KEYWORDS/DESCRIPTORS</small> <table style="width: 100%;"> <tr> <td style="width: 50%;"> Low-Level waste Source Term modeling Unsaturated water flow Metallic container degradation </td> <td style="width: 50%;"> Waste form leaching Unsaturated Contaminant Transport </td> </tr> </table>				Low-Level waste Source Term modeling Unsaturated water flow Metallic container degradation	Waste form leaching Unsaturated Contaminant Transport	<small>15. AVAILABILITY STATEMENT</small> Unlimited			
Low-Level waste Source Term modeling Unsaturated water flow Metallic container degradation	Waste form leaching Unsaturated Contaminant Transport								
<small>b. IDENTIFIERS/OPEN-ENDED TERMS</small>				<small>16. SECURITY CLASSIFICATION</small> <small>(This page)</small> Unclassified <small>(This report)</small> Unclassified					
<small>17. NUMBER OF PAGES</small> 327				<small>18. PRICE</small>					

Property of
GNWRA Library

19/29
NUREG/CR-5387
BNL-NUREG-52206
RW

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

DCOM
Manuscript Completed: May 1989
Date Published: July 1989

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

Brookhaven National Laboratory
Upton, NY 11973

T 199708060002
Prepared for
Division of Engineering
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
NRC FIN A3276

20/29

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 form 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.

21/29

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 are 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 input 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

	<u>Page</u>
ABSTRACT	iii
EXECUTIVE SUMMARY.	v
LIST OF FIGURES.	ix
LIST OF TABLES	xi
 1. INTRODUCTION AND BACKGROUND	 1
2. PRINCIPLES OF MODELING GROUNDWATER FLOW -- AN OVERVIEW.	3
2.1 Methodology.	3
2.2 The Governing Equation	4
2.3 Initial and Boundary Conditions.	6
2.4 Assumptions and Limitations in FEMWATER.	8
3. BLT - BREACH, LEACH, AND TRANSPORT.	9
3.1 Container Degradation (BREACH)	9
3.2 Release of Radionuclides from the Waste Form (LEACH)	12
3.2.1 Diffusion Release	13
3.2.2 Dissolution Release	21
3.2.3 Rinse Release	22
3.2.4 Total Release Rate.	22
3.3 Radionuclide Migration (TRANSPORT)	23
3.3.1 Governing Equation for Contaminant Transport in the Unsaturated Zone.	 24
3.3.2 Initial and Boundary Conditions	26
3.4 Limitations in the BLT code.	27
4. COUPLING BETWEEN THE MAJOR PROCESS MODELS	29
5. PROCEDURES AND INPUTS FOR FEMWATER.	33
5.1 Procedures	33
5.2 Input Information.	33
5.2.1 Basic Parameters.	33
5.2.2 Compressibilities and Hydraulic Properties.	34
5.2.3 Elemental and Nodal Information	34
5.2.4 Initial and Boundary Conditions	34
6. APPLICABILITY OF THE COUPLED FEMWATER-BLT CODES	37
6.1 Applications	37
6.2 Limitations.	38
6.3 An Example of Application of FEMWATER.	39

24/29

CONTENTS (continued)

	<u>Page</u>
6.3.1 Geometry of a Shallow Land Burial Trench.	39
6.3.2 Boundary Conditions	40
6.3.3 Soil Properties	42
6.4 Results and Discussions.	42
6.5 Examples of BLT Application.	45
6.5.1 Set-up for BLT.	45
6.5.2 Case Examples	51
7. ANNOTATED INPUT GUIDE FOR FEMWATER.	53
8. BLT DATA INPUT GUIDE.	87
8.1 Data Input Guide for BLT	87
8.2 Annotated Input Deck for BLT	131
8.3 BLT Output	140
9. REFERENCES.	159
APPENDIX 1: Hydraulic Conductivity and Permeability.	161
APPENDIX 2: Soil Properties in the Unsaturated Zone.	173
APPENDIX 3: Mass-Volume Relationships.	209
APPENDIX 4: An Example of Automatic Numbering of Element Incidences.	213
APPENDIX 5: Initial and Boundary Conditions.	215
APPENDIX 6: Variable Array Dimensioning.	217
APPENDIX 7: Data Requirements for the Breach Model	225
APPENDIX 8: Data Requirements for the Leach Model.	231
APPENDIX 9: Data Requirements for the Transport Equation	243
APPENDIX 10: BLT Graphics Files	249
APPENDIX 11: Typical Low-Level Waste Inventory Data	253
APPENDIX 12: Redimensioning the finite element grid for the transport calculation in BLT, REDIMGRD.EXE.. . . .	275
APPENDIX 13: Restart Capabilities in BLT.	277
APPENDIX 14: FEMWATER Printer Output File Example	283
APPENDIX 15: BLT Program Structure.	319

46/80/4
at

25/29

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 Sullivan, Group Leader
Performance and Risk Assessment

TS:al

Nov 20, 97 16:16

randy.tjm

Page 1/1

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	Fraction for Rinse#1	Diffusion Rate (ft**2/year)	Fraction for diff.	Dissolution Rate (ft/year)	Fraction for dis.	Dis. Radius (feet)
'A6	0.800E+00	3.000E-07	0.200E+00	6.200E-04	0.000E+00	5.000E-02
'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

6/9/97

[illegible]

```
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            *
C * FOR THE ACCURACY, COMPLETENESS OR USEFULNESS OF ANY INFORMATION,               *
C * APPARATUS, PRODUCT OR PROCESS DISCLOSED, OR REPRESENTS THAT ITS USE           *
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 UNSATURATED, FRACTURED                    *
C *                   MEDIA.                                                 *
C *                             *                                                *
C *   LANGUAGE      -   ANSI STANDARD FORTRAN, VERSION77                    *
C *                             *                                                *
```

29/29

```
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                        *
C *                   EVARISTO J. BONANO                     *
C *                   *
C *****
```