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

> 9103050503 910228 PDR NUREG CR-5618 R PDR

AVAILABILITY NOTICE

Availability of Reference Materials Cited in NRC Publications

Most documents cited in NRC publications will be available from one of the following sources:

- 1. The NRC Public Document Room, 2120 L Street, NW, Lower Level, Washington, DC 20555
- The Superintendent of Documents, U.S. Government Printing Office, P.O. Box 37082, Washington, DC 20013-7082
- 3. The National Technical Information Service, Springfield, VA 22161

Although the listing that follows represents the majority of documents olded in NRC publications, it is not intended to be exhaustive.

Referenced documents available for inspection and copying for a tee from the NRC Public Document Boom include NRC correspondence and internal NRC memoranda; NRC Office of inspection and Enforcement bulletins, sinculars, information notices, inspection and investigation notices; Licensee Event Reports; vendor reports and correspondence; Commission papers; and applicant and licensee documents and correspondence.

The following documents in the NUREG series are available for purchase from the GPO Sales Program: formal NRC staff and contractor reports, NRC-sponsored conference proceedings, and NRC booklets and brochures. Also available are Regulatory Guides, NRC regulations in the Code of Federal Regulations, and Nuclear Regulatory Commission Issuances.

Documents available from the National Technical Information Service Include NUREG series reports and technical reports prepared by other federal agencies and reports prepared by the Atomic Energy Commission, forerunner agency to the Nuclear Regulatory Commission.

Documents available from public and special technical libraries include all open literature items, such as books, journal and periodical articles, and transactions. *Federal Register* notices, federal and state legislation, and congressional reports can usually be obtained from these libraries.

Documents such as theses, dissertations, foreign reports and translations, and non-NRC conference proceedings are available for purchase from the organization sponsoring the publication cited.

So gle copies of NHC draft reports are available free, to the extent of supply, upon written request to the Office of Information Resources Management, Distribution Section, U.S. Nuclear Regulatory Commission, Washington, DC 20555.

Copies of industry codes and standards used in a substantive manner in the NRC regulatory process are maintained at the NRC Library, 7920 Norfolk Avenue, Bethesda, Maryland, and are available there for reference use by the public. Codes and standards are usually copyrighted and may be purchased from the originating organization or, if they are American National Standards, from the American National Standards Institute, 1430 Broadway, New York, NY 10018.

DISCLAIMER NOTICE

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability of responsibility for any third party's use, or the results of such use, of any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights.

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. 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

Untera, 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 11 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 timedependent velocity fields, 3) the ability to account for the effect of time-dependent saturation changes on the retardati n 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.

ť,

TABLE OF CONTENTS

1.0	INTR	ODUCTIO	8	1-1
	$\begin{matrix}1.1\\1.2\\1.3\end{matrix}$	Backgr Purpos Report	ound e Structure	$1 - 1 \\ 1 - 1 \\ 1 - 3$
2.0	DESC	RIFTION	OF MODELS	2 - 1
	2.1	Networ	k Flow Model	2 - 2
		2.1.1 2.1.2 2.1.3	Theory Implementation Fluid Density and Viscosity Submodels	2 - 2 2 - 3 2 - 5
	2.2	Analyt	ical Transport Model	2 - 7
		$\begin{smallmatrix}2&.2&.1\\2&.2&.2\end{smallmatrix}$	Theory Implementation	2 - 8 2 - 8
	2.3	Source	Model	2-12
		$\begin{smallmatrix}2&,3&,1\\2&,3&,2\end{smallmatrix}$	Theory Implementation	2-13 2-18
	2.4	Distri	outed Velocity Method (DVM) Transport Model	2 - 21
		$\begin{array}{c} 2.4.1 \\ 2.4.2 \\ 2.4.3 \\ 2.4.4 \\ 2.4.5 \\ 2.4.6 \\ 2.4.7 \\ 2.4.8 \\ 2.4.9 \\ 2.4.10 \\ 2.4.11 \end{array}$	Theory	2 - 21 2 - 25 2 - 33 2 - 35 2 - 36 2 - 47 2 - 49 2 - 50 2 - 54 2 - 59
3.0	DESC	RIPTION	OF CODE	3-1
	3.1	Structu	1Fe	3-1
		3.1.1 3.1.2 3.1.3	General Source Module Transport Module	3 - 1 3 - 3 3 - 3

TABLE OF CONTENTS

233.2

	3.2	Subroutines	3-3
		3.2.3 NEFMAIN , main program	1.6
		3.2.7 ADTRIVA TO TO TO TIACH PUT	1.6
		2.3.3 BAND/PETADE EPUDA	3.0
		3.5 & RDANOU/PDES	3.9
		2.5.6 BONTHEFTERS	2-1-
		DIGID DOULYE(ADB) IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	3 - 7
		3.5.7 CHATRIAN NEL VOL CONTRACTOR CONTRACTOR	3-7
		3.6.7 WRAIN(1W) CONTRACTORES CONTRACTORES CONTRACTORES	3 - 7
		3.2.6 URKPIR TREASUREMENTATION CONTRACTOR CONTRACTOR	3+8
		3.6.Y SUBFE CONTRACTOR CONTRACTON	3+8
		DIGINO DEVERT ANALYSIA CONTRACTOR CONTRACTOR CONTRACTOR CONTRACTOR	3 + 8
		Sidika DADT verification entreter entre	3+8
		Julik ET entrementerenterenterenterenterenterente	3-9
		J.K.IJ FAGER ALTERTATION CONTRACTOR CONTRACTOR A	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)	1.14
		3.2.28 SOURCE(IFASS, JTRIAL)	3-14
		3.2.29 SRCIN(T, SR1, SR2, TS1, TS2, N1, N2, NTOTX, S24, IEOF) 3	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, FDIS)	3-17
		3.2.34 TRNSPT(T, TSET, NTF, 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	1.19
	3.4	Common Blacks	3.20
		And and an and a second s	
0	DATA	INPUT GUIDE	4-1
	4.1	Execution Procedure for NEFTRAN II 4	4-1
	4,2	General Input Description 4	4+2
	4.3	Parameter Input Description 4	4 + 3
		1.2.1. 000000	
		HIGH OPTIONS ANTAL CONTRACTOR CONTRACTOR CONTRACTOR CONTRACTOR	5 - 3
		4.3.2 Froblem Size Farameters	4 - 1 0

4.

TABLE OF CONTENTS

Page

		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 #	lequired for Multiple Simulations	4-29
		4.5.1	Multiple Data Sets	4-29
		4.5.2	Use of Subroutine GETRV	4-31
			NOR DE DEDEDEDEDE COMPANY CONTRACTOR CONTRAC	
	4.6	Sample	Input File	4-31
5.0	VER	FICATIO	ON AND SAMPLE PROBLEMS	5-1
	5.1	Samp14	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
	TO DO	IN DALOP O		11
0.0	KEFI	SKENCES.	· 医甲基甲基卡弗里诺 医洗子 医单元子 有关 医子子 医注释 医子子 医马克特 医子子 医子子 医子子 医子子 医子子 医子子	0-1
APPE	NDIX	A 5	Species Velocity Model	A - 1
APPE	XIDN	B I	Discharge Model	B - 1
APPE	NDIX	C I	Distribution of Source Into Migration Path	
			using mixing-bell Model	C - 1
APPE	NDIX	D S	Storage of Decay Chain Information	D - 1
APPE	NDIX	E C	Output Files for Sample Problems	E-1

LIST OF FIGURES

-			
- 12	а.	- 14	
		- 60	
- 6			
		-	

2.1. 2.2. 2.3. 2.4. 2.5	Illustration of Conservation of Mass at a Junction Example Flow Network for Use in NEFTRAN II The Mixing Cell The Spatial Green's Function	2 - 2 2 - 6 2 - 17 2 - 24
2.6.	Point Source Illustration of the Mixing Fraction Concept Example Breakthrough Curves (NEFTRAN II,	2 - 26 2 - 29
2.8.	Analytical Solution) Example Breakthrough Curves with Concentration	2-38
2.9.	on a Logarithmic Scale Comparison of Finite Difference Solution to Analytical	2-40
2.10.	Solution	2-41
2.11	1.0 x 10 ⁵ y	2-43
2.12.	Discharge Rate Curves for Problem Simulation Time *	2-45
2.13.	Illustration of Four Possible Situations Arising Because	2-66
2.14.	Illustration of Adjacent System of Grid Blocks Simulating	2-55
	the Rock Matrix in Dual-Porosity Legs	2 - 57
3.1. 3.2. 3.3.	General Flowchart of NEFTRAN II Flowchart of Source Module in NEFTRAN II Flowchart of Transport Module in NEFTRAN II	3 - 2 3 - 4 3 - 5
5.1. 5.2. 5.3.	Physiographic Setting of the Reference Site Reference Site Geology Ground-Water Flow at Reference Site	5-2 5-3 5-4
5.5. 5.6.	SWIFT II Gridding for the Reference Site	5-7
5.7.	(Dark Lines Indicate Network Legs)	5-8 5-9
5.8.	233U Discharge Rates for Sample Problem #1	5-21
5.10.	Breakthrough Curve for Sample Problem #2	5-23
5.12.	Discharge Rate Curves for Sample Problem #3	5.35

LIST OF FIGURES

0

Page

"。 "你为什

1

B.1	Total and Partial Discharge of a Typical Velocity Packet	B - 2
0.1	The Grid Block Numbering Convention	C - 3
C.2	Shaded Area Represents the Region of Integration for Total Source of Species 2 from Species 1	C - 6
¢.3	Possible Integration Regions for the Case ν_1 - ν_2	C - 8
0.4	The Possible Regions of Integration for Subcase 2.1	C-11
6 .5	Regions of Integration for Subcase 2.2	C-14
C.6	Regions of Integration for Subcase 2.3	C-16

-1x-

.

LIST OF TABLES

Page

2.1.	Boundary and Initial Conditions for the Analytical	
	Solution Transport Model	2-9
8.2.	Parameters for Example Problem	2-42
4.1.	Input Template for Standard Print Options	4.4
4.2.	Input Template for External File Options	4-7
4.3.	Input Template for Run Control Ontions	4.8
4.4.	Input Template for Debug Print Ontions	4.10
4.5.	Input Template for Problem Size Parameters	4-10
4.6.	Input Template for Source/Flow Parameters	4-16
4.7.	Input Template for Time Parameters	4-15
4.8	Input Templete Fur Increment Determination Parameters	4-10
4.9	Recommended Sets of Values for the Increment.	4.10
610.1	Determination Parameters	1.10
4.10.	Input Template for Network Les Properties Arres	4-17
4.11.	Input Template for Network Junction Properties Arres	4-21
4.12	Input Template for Migration Dath Properties Array	4-26
4.13	Run Option Combinations	4-22
4.14	Mipration Darh Array Davamatava as a Dunation of	4-23
	Run Option	2 41
4.15	Innut Template for Decay Chaine Arrey	4-24
4.16	Input Template for Flement Despective Areas	4-28
4.17	Input Template for Multiple Date Fot Options	4-29
4.18	Sample Input File	4-30
4.20.	Sembre rubne trretterstation to the state of	4-32
5.1.	Input File for Sample Problem #1	5-10
5.2.	Reference Site Hydraulic Properties	5.17
5.3.	Input File for Sample Problem #2	5.97
5.4.	Input File for Sample Problem #3	5.31
5.5.	External File of Time-Varving Velocity Data	5.33
	second the of the solying feroutly baca minimum	3-93
C.1	Integration Limits Needed to Evaluate Equation C.14	
	for Subcase 2.1	C-12
C.2	Integration Limits Needed to Evaluate Equation C.14	
	for Subcase 2.2	C-13
0.3	Integration Limits Needed to Evaluate Equation 6.14	
	for Subcase 2.3	C-17

ACKNOWLEDGMENT

The authors wish to express their thanks to David Callegos, Phil Pohl, Ron DyKhuizen and Tim McCartin for their review of this document, and to Ms. Irene Gonzales for her hard work in typing this document. They would also like to thank Dr. Evaristo Bonano for his support and consultation on the development of NEFTRAN II and for reviewing this document.

1.0 INTRODUCTION

This report describes the NEFTRAN II (<u>NE</u>twork Flow and <u>TRAN</u>sport in Time-Dependent Velocity Fields) computer code developed by Sandia National Laboratories (SNL) for the U.S. Nuclear Regulatory Commission (NRC). The following sections discuss pertinent background concerning the NEFTRAN II computer code, the purpose of developing the code, and the structure of this report.

1.1 Background

NEFTRAN II is the fourth in a family of codes developed by SNL for the NRC. Predecessors to NEFTRAN II are NEFTRAN (Longsine and others, 1987), NWFT/DVM (Campbell and others, 1981b), and NWFT (Campbell and others, 1979). These codes have evolved such that each new version contains all the capabilities of its immediate predecessor in addition to new features. NWFT and NWFT/DVM were developed as a tool to help the NRC assess the performance of high-level radioactive waste disposal sites in geologic media. Specifically, NWFT and NWFT/DVM were used to simulate radionuclide ground-water transport through saturated porous media from a repository to a discharge point. With NEFTRAN, the capability to simulate transport through saturated dual-porosity or fractured media was added. In NEFTRAN II, the capability to transport radionuclides through time-dependent velocity fields, which may be applied to simulate transport in unsaturated media, has been added. NWFT changed as (1) the sites considered for HLW disposal changed, (2) the analyses required to apply for licensing and assessing a license evolved, and (3) the standards for HLW disposal and analyses required to prove compliance with those standards evolved. 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.

1.2 Purpose

The purpose of the NEFTRAN II computer code is to simulate radionuclide transport in ground water as part of a performance assessment methodology for a high-level radioactive waste repository. In the performance assessment methodology, a large number of simulations are required to address parameter uncertainty and sensitivity. Furthermore, since the performance measure for a HLW repository in the U.S. is integrated discharge to the accessible environment at 10000 years, relatively long simulation times are required. Consequently, the radionuclide transport code for use in a performance assessment methodology must be computationally efficient, as well as being able to simulate the transport of multiple radioactive chains with multiple members. NEFTRAN II and its predecessors were developed to meet these performance assessment requirements.

There are several ways in which NEFTRAN II can be used in a performance assessment methodology. For a saturated, steady-state flow field, the network flow model contained in NEFTRAN II can be used in conjunction with a detailed flow model such as that contained in the SWIFT II code (Reeves and others, 1986a, 1986b). The mathematical models in the SWIFT II code are based on the assumption that the medium in which flow and transport are occurring is continuous, which may lead to a fully mul' dimensional flow system. The flow and transport models contained 1% NEW RAN II are based on the assumption that all significant flow and radionuclide transport takes place along pathways that can be simulated as discrete one-dimensional legs or paths. These legs are assembled to form a multi-dimensional network representation of the flow field. To define this network representation and the migration path, the results of a detailed flow model (such as the one contained in SWIFT II), and a particle-tracking method (such as the one used by Bonano and others, 1989) can be used. The particle tracking method is used to define the trajectory that a tracer particle released from a given point (e.g., the repository) will follow until it crosses some prescribed boundary (e.g., the accessible environment) in the flow field predicted by SWIFT II. Based on the particle tracking model and the flow field predicted by SWIFT II the length, location of end points, cross-sectional area, migration path, and all hydraulic properties of each leg in the network flow system can be defined. With the appropriate boundary pressures from SWIFT II, the network can reproduce the flow field. As long as this reproduction remains valid under statistical variation, the use of a network to define the flow field makes NEFTRAN II a more computationally efficient code than codes like SWIFT II and therefore, for the multiple simulations required for performance assessment, using NEFTRAN II is more practical.

NEFTRAN II can also be used in a performance assessment methodology without utilizing the network flow model (i.e., without modeling flow), by direct input of pore velocities into the transport model. In this case NEFTRAN II can be coupled with a flow model such as the one contained in DCM3D (Updegraff and Lee, 1991), which simulates flow in unsaturated, fractured media. Again, a particle tracking-method would be used to determine a dominant one-dimensional transport path for NEFTRAN II from the results of DCM3D. Significant changes in pore velocities and saturations with time along this path can also be determined from a detailed flow model such as the one contained in DCM3D and then utilized by NEFTRAN II for the radionuclide transport analysis. The underlying assumption is that the flow path is essentially constant with time and only the magnitude of the velocity is time-dependent.

Although NEFTRAN II is designed for a performance assessment methodology, it can be used for general analysis of radionuclide transport in ground water and can be run easily by a wide variety of users. NEFTRAN II may appear extremely simple to use, but applying it to a problem, and the meaning of the results obtained, requires as much thought and analysis as using what might appear to be a more complex code. For this reason, the user must have knowledge of flow and transport through porous media and must be able to discern when the models contained in NEFTRAN II are adequate for the problem being simulated. The purpose of this report is not to tell the user when to use NEFTRAN II, but rather how to use NEFTRAN II once the user has decided the models that it contains are appropriate for the specific problem being simulated.

1.3 <u>Report Structure</u>

The structure of this report is as follows. Chapter 2 describes the models contained in NEFTRAN II, which includes the network flow model. the analytical transport model, the source model, the distributed velocity method (DVM) transport model, and the matrix diffusion 4el. Chapter 3 describes the code structure, the parameter statements . in the code, the common blocks used in the code, and the subroutines contained in the code. Chapter 4 is a data input guide, and verification and sample problems are presented in Chapter 5. For the first time user, it is recommended that Chapters 2, the first section of Chapter 3, Chapter 4 and Chapter 5 be read initially, since the last three sections of Chapter 3 and the appendices are a more detailed description of the actual code and may be of more utility as the user gains experience with the code. Special attention should be paid to sections 2.4.3 and 2.4.4 which describe the criteria for space- and time-increment determination. The numerical criteria for the DVM numerical technique used in NEFTRAN II are substantially different from other numerical transport schemes and must be understood before the code can be used properly.

2.0 DESCRIPTION OF MODELS

The following sections describe the flow, source, and transport models contained in NEFTRAN II. The theoretical basis for each model, as well as numerical implementation, is discussed.

The first step is to define the ground-water flow path and, if necessary, the ground-water flow rate through the source region. These can be defined in one of three ways:

- specify the geometric and hydraulic properties of a flow network in the standard NEFTRAN II input file (described in Section 4) and use the network flow model (described in Section 2.1) to solve for the pressures, flow rates and velocities,
- input pore velocities and source flow retas via the standard NEFTRAN II input file, or
- input pore velocities and source flow rates from external files (described in Section 2.4.11 and Section 2.3.2). This option was designed to allow for time-dependent flow behavior when simulating radionuclide transport.

After defining the ground-water flow path, the next step is to simulate radionuclide transport.

Section 2.2 contains the theory and implementation for an analytical solution to the convective dispersion transport equation. This solution is restricted to (1) decay chains having no more than three members, (2) each member of the decay chain must have identical retardation factors, (3) a steady-state flow field, and (4) the source must be equivalent to a concentration boundary condition. This analytical solution, coupled with a network flow model (fixed number of legs and junctions), comprised the NWFT model (Campbell, and others, 1979).

Introduction of the distributed velocity method (DVM) (Campbell and others, 1980) for radionuclide transport into NWFT resulted in the second code of the sequence, NWFT/DVM (Campbell and others, 1981a, 1981b). With DVM, many limitations imposed by use of the analytical solution were eliminated by allowing the consideration of radionuclide chains of arbitrary length, the members of which could have significantly different retardation factors. Most of the capabilities of NWFT/DVM, NEFTRAN (Longsine and others, 1987) and NEFTRAN II, center around the DVM technique. For example, the source model (described in Section 2.3) was developed specifically for DVM and the matrix diffusion model (Section 2.4.10) is directly coupled to DVM. The capability to transport radionuclides in time-dependent velocity fields (discussed in Section 2.4.11) is also directly coupled to the DVM transport model. None of these models can be used with the analytical transport solution.

2.1 Network Flow Model

2.1.1 Theory

In the flow-network model, the driving force for flow through a leg is a pressure gradient. Consequently, the network flow model contained in NEFTRAN II can be used to simulate saturated ground-water flow. The flow network is used to represent a saturated flow system by solving the conservation-of-mass equation at each junction. This principle can be expressed mathematically as

$$\Sigma_{I}M_{I} = 0$$
, (2.1)

where the sum is over all legs connected at the given junction, and M, is the mass flow rate for the ℓ^{th} leg in units of mass per unit time. Flow rates into the junction are considered positive and flow rates out of the junction are considered negative. Figure 2.1 illustrates this principle for three legs surrounding a junction.

For this simple example, Equation 2.1 becomes

$$M_1 + M_2 - M_3 = 0$$
 (2.2)
 $M_1 + M_2 = M_3$.

or





If the *l*th leg is bounded by Junctions *l*1 and *l*2, the mass flow rate in the leg is defined by

$$M_{\hat{g}} = \rho_{\hat{g}} K_{\hat{f}} A_{\hat{f}} \left[\frac{(P_{\hat{f}1} - P_{\hat{f}2})}{Z_{\hat{f}} \rho_{\hat{f}} g} + \frac{(E_{\hat{f}1} - E_{\hat{f}2})}{Z_{\hat{f}}} \right] , \qquad (2.3)$$

where A, is cross-sectional area (length²), K is hydraulic conductivity (length/time), E_{f1} is elevation of the 1th junction, g is the acceleration of gravity (length/time²), P_{f1} is pressure (force/area) at the 1th junction, Z is length of the leg, and ρ_f is fluid density (mass/volume). Equation 2.3 incorporates the sign convention that M is positive if the flow direction is from Junction fl to Junction f2. The hydraulic conductivity is weighted as

$$K_{\underline{\ell}} = K_{\underline{\ell}}' \left[\frac{\mu_{\underline{\ell}}}{\mu_{\underline{\ell}}} \right] \left[\frac{\rho_{\underline{\ell}}}{\rho_{\underline{\ell}}} \right]$$

(2.4)

to account for the effects of brine concentration on the flow; K' is the fresh-water hydraulic conductivity for the $\ell^{\rm th}$ leg, μ_ℓ and ρ the viscosity (mass/length/time) and density of fresh water at approximately 20°C, and μ_ℓ and ρ_ℓ are the actual viscosity and density of the brine solution in the $\ell^{\rm th}$ leg. The manner in which μ_ℓ and ρ_ℓ are determined in NEFTRAN 11 is discussed in Section 2.1.3.

Equation 2.3 is a mathematical statement of Darcy's law in which the total head difference is given by the sum of dynamic pressure and elevation differences. This equation typically has three unknowns M_{g} , P_{g1} , and P_{g2} , unless either Junction 11 or Junction 12 has been specified as a boundary junction with known pressure. For each junction in the network, Equation 2.1 is written and Equation 2.3 is substituted for M. This eliminates the mass flow rates as unknowns leaving only the junction pressures to be determined since the elevations are supplied as part of input.

2.1.2 Implementation

Based on the above discussion, NEFTRAN II implements the network flow model by applying Equation 2.1 to a generalized flow network system. For example, if Figure 2.1 is part of a larger network, applying Equation 2.1 to Junction 3 in Figure 2.1, and substituting Equation 2.3 for M, gives

where $\theta_{\ell} = A_{\ell}K_{\ell}/Z_{\ell}g$. Repeating this process for every junction in the network results in a matrix equation of the form,

which can be written using matrix notation as

$$\frac{\Theta}{m} = \frac{E}{2}$$
, (2.7)

where Θ is the matrix of coefficients, p the vector of unknown

pressures, and g the vector of junction elevations and boundary pressures representing the right-hand side of Equation 2.5. The dimension of the matrix equation is the number of junctions having unknown pressure.

After solving for the junction pressures, NEFTRAN II calculates the mass flow rate in each leg using Equation 2.3 and divides by the corresponding density to determine the volumetric flow rate. The volumetric flow rate is used to obtain the average fluid velocity for each leg along the radionuclide migration path used by the transport models in NEFTRAN II. Specifically, from Equation 2.3.

$$Q_{\ell} = \kappa_{\ell} \Lambda_{\ell} \left[\frac{\left[P_{\ell 1} - P_{\ell 2} \right]}{Z_{\ell} \rho_{\ell} g} + \frac{\left[E_{\ell 1} - E_{\ell 2} \right]}{Z_{\ell}} \right] , \qquad (2.8)$$

where Q is the volumetric flow rate (volume/time) in the 1th leg. The average fluid pore velocity (length/time) in the leg is

$$v_{\ell} = \frac{Q_{\ell}}{A_{\ell}\phi_{\ell}} , \qquad (2.9)$$

where ϕ_{j} is the effective porosity (dimensionless).

In NEFTRAN II, Equation 2.7 is solved using a special case of the Gaussian elimination technique designed for banded matrices. For efficiency, the user should keep the band width as small as possible. Except for boundary junctions with known pressures, this means that the junction numbers surrounding a given junction should be close to the given junction number. In fact, if Junctions &1 and &2 are connected by a leg, dimensioning statements in the code require $|l1 - l2| \leq 5$.

The network flow model in NEFTRAN II allows the user to represent any flow network by specifying the hydraulic properties of each network leg, the junctions bounding the leg, junction elevations, and the known pressures at the boundary junctions. Figure 2.2 shows an example flow network for use in NEFTRAN II to simulate saturated ground-water flow. Horizontal legs might represent different geological strata while vertical legs could represent potential pathways for hydraulic communication between layers. In this example, the user would have to specify pressures at Junctions 1, 2, and 3, as these are boundaries in the flow network.

2.1.3 Fluid Density and Viscosity Submodels

Fluid density and viscosity (ρ_g and μ_g) are needed for the network flow model, as defined in Equations 2.3 and 2.4. In reality, water density and viscosity are functions of temperature, pressure, and brine concentration. However, the dependence of water density and viscosity on pressure has been found to be negligible (Cranwell and others, 1982). Furthermore, NEFTRAN II was designed to simulate transport processes under isothermal conditions. Thus, water density is assessed to be a function of brine concentration only. Specifically, water density is assumed to be a linear function of brine concentration; i.e.,

$$\rho(C) = \rho_{f} + C \left[\rho_{e} - \rho_{f} \right] , \qquad (2.10)$$

where C is the dimensionless brine concentration (C = 0 for fresh vater and C = 1 for saturated brine), $\rho_{\rm f}$ the density of fresh water at reference temperature (62.3 lb/ft³ at 68°F), and $\rho_{\rm s}$ the density of saturated brine at the reference temperature (74.02 lb/ft³ at 68°F). Equation 2.10 is used to determine the fluid density for each network leg based on the relative brine concentration (C) of each leg.

The dependence of viscosity on concentration of dissolved solids can be approximated as

$$\mu(C) = \mu(0) \left[1.0 + 0.005 \int_{i=1}^{N} c_i + \sum_{i=1}^{N} A_i c_i \right] , \qquad (2.11)$$

where c_i is the concentration dissolved ion (i) in moles/liter, Λ_i the temperature dependent coefficient, $\mu(0)$ the viscosity of fresh water at 68°F, and N the number of dissolved species.

For ground-water systems, solutions containing more than 10 or 15 moles/liter of dissolved ions are unlikely; therefore, the square root term in Equation 2.11 can be neglected. Assuming NaCl is the primary dissolved mineral, then N = 2 and the dissolved species are Na^{*} and Cl^{*}.



Figure 2.2. Example Flow Network for Use in NEFTRAN II

For these ions, the coefficients (A) can be assumed to be independent of temperature, and are defined as

$$A(C1) = 0$$

and

 $A(Ne^+) = 0.08$.

Given these arguments, Equation 2.11 can be simplified to

$$\mu(C) = \mu(0) \left[1.0 + 0.08 c(Na^{+}) \right] . \qquad (2.12)$$

The concentration of dissolv_d Na* is given as

$$c(Na^{+}) = W \left(\frac{1b \text{ salt}}{1b \text{ sol}}\right) \cdot C \cdot \rho \left(\frac{1b \text{ salt}}{ft^{3} \text{ sol}}\right)$$
$$\cdot 454 \left(\frac{gm}{1b}\right) \cdot \left(\frac{1}{2.83 \times 10^{4}}\right) \left(\frac{ft^{3}}{cm^{3}}\right) 1000 \left(\frac{cm^{3}}{l}\right) \qquad (2.13)$$
$$\cdot \left(\frac{1}{58.443}\right) \left(\frac{\text{moles NaCl}}{gm}\right) \quad ,$$

where W is the weight fraction of salt in saturated brine, C the dimensionless brine concentration, and ρ (= ρ (C)) the density of brine at concentration C (from Equation 2.10).

Thus, Equation 2.12 becomes

$$\mu(C) = \mu(0) [1.0 + 0.0219 WCp]$$
(2.14)

Equation 2.14 is use ". NEFTRAN II to estimate fluid viscosity for each leg in the flow network based on the relative brine concentration (C) within the leg.

2.2 Analytical Transport Model

The analytical transport model that formed the basis for NWFT has been retained in each of its successors. The theory and implementation for this model is discussed in the following subsections.

2.2.1 Theory

NEFTKAN II contains two models that can simulate radionavide transport. The analytical transport option simulates the migration of a three-member radioactive decay chain in a one-dimensional constant velocity system, as described by the following differential equations:

$$R = \frac{\partial N_1}{\partial t} = D = \frac{\partial^2 N_1}{\partial x^2} - v = \frac{\partial N_1}{\partial X} - R = \lambda_1 N_1 \qquad (2.15)$$

$$k \frac{\partial N_2}{\partial t} = D \frac{\partial^2 N_2}{\partial x^2} + v \frac{\partial N_2}{\partial x} + R \lambda_2 N_2 + R \lambda_1 N_1 \qquad (2.16)$$

$$R \frac{\partial N_3}{\partial t} = D \frac{\partial^2 N_3}{\partial x^2} - v \frac{\partial N_3}{\partial x} - R \lambda_3 N_3 + R \lambda_2 N_2 , \qquad (2.17)$$

where R is the constant retardation factor (dimensionless) that is assumed to be equal for all three radionuclides, N_i the concentration (mass/volume) in solution of species i, D (= $|v| \alpha$) the dispersion coefficient (length²/time), α the dispersivity (length), λ_i (= $\ln 2/T_{1/2}$) the decay constant for species i (time⁻¹), and $T_{1/2}$ the half-life for species i (time).

Equations 2.15 - 2.17 represent conservation of mass for a species in a differential volume. The left-hand side (LHS) in each of these equations denotes the rate of change of dissolved species within this volume. The terms in the right-hand side (RHS) represent the flux of species in and out of the volume, and the source/sink terms within the volume. Specifically, the first and second terms in the RHS stand for the net flux of the species by mechanical dispersion and convection, respectively while the last two terms represent production and depletion of the species due to radioactive decay.

The boundary conditions and initial condition used in conjunction with Equations 2.15, 2.16, and 2.17 are listed in Table 2.1. Based on these conditions, the source for the analytical transport model is a concentration boundary condition and the source model discussed in Section 2.3 is not implemented when the user selects the analytical transport model.

2.2.2 Implementation

To implement the analytical solution transport model in NEFTRAN II, the analytical solution for Equations 2.15, 2.16 and 2.17 with the indicated initial and boundary conditions is utilized. The time-dependent discharge rates predicted by Equations 2.15, 2.16, and 2.17, as given by Lester, Jansen, and Burkholder (1975), are

Table 2.1.

Boundary and Initial Conditions for the Analytical Solution Transport Model

I. $\frac{t = 0, all x}{C_1 = C_2 = C_3} = \dots = 0$ 0 < t < r, x = 0II. $C_1 = \frac{N_1(0)}{Or} e^{-\lambda_1 t}$ $C_2 = \frac{N_2(0)}{Qr} e^{-\lambda_2 t} + \frac{\lambda_1}{\lambda_2 - \lambda_1} \frac{N_1(0)}{Qr} \left(e^{-\lambda_1 t} - e^{-\lambda_2 t} \right)$ $C_{3} = \frac{N_{3}(0)}{Qr} e^{-\lambda_{3}t} + \frac{\lambda_{2}}{\lambda_{3}-\lambda_{2}} \frac{N_{2}(0)}{Qr} \left(e^{-\lambda_{2}t} - e^{-\lambda_{3}t} \right)$ $+ \lambda_1 \lambda_2 \frac{N_1(0)}{Qr} \frac{e^{-\lambda_1 t}}{(\lambda_2 \cdot \lambda_1)(\lambda_3 \cdot \lambda_1)} + \frac{e^{-\lambda_2 t}}{(\lambda_1 \cdot \lambda_2)(\lambda_3 \cdot \lambda_2)} +$ $\frac{e^{-\lambda_3 t}}{(\lambda_1 \cdot \lambda_3)(\lambda_2 \cdot \lambda_3)}$ III. $\frac{t > r, x = 0}{C_1 = C_2 = C_2} = \dots = 0$

IV. $\frac{t > 0, x \to \infty}{C_1, C_2, C_3, \dots} = finite$

 $N_1(0)$ is the initial inventory of species i, Q the fluid flow rate, and τ the leach rime for a constant leach rate source.

$$D_{1}(t) = \frac{N_{1}(0)}{2r} \cdot \lambda_{1}t [(U(t) - U(t - r)H(t - r))]$$
(2.18)

$$D_{2}(t) = \left[\frac{N_{2}(0) e^{-\lambda_{2}t}}{2r} + \frac{N_{1}(0)}{2r} \left(\frac{\lambda_{1}}{\lambda_{2} - \lambda_{1}} \right) \left[e^{-\lambda_{1}t} e^{-\lambda_{2}t} \right] \right]$$

$$\left[\left[(U(t) - U(t - r)H(t - r)) \right]$$

$$(2.19)$$

$$5^{(\tau)} = \left[\frac{N_3(0)}{2\tau} e^{-\lambda_3 t} + \frac{N_2(0)}{2\tau} \left(\frac{\lambda_2}{\lambda_3 \cdot \lambda_2} \right) \left(e^{-\lambda_2 t} e^{-\lambda_3 t} \right) \right]$$

$$+ \frac{N_1(0)}{2\tau} \lambda_1 \lambda_2 \frac{e^{-\lambda_1 t}}{(\lambda_2 \cdot \lambda_1)(\lambda_3 \cdot \lambda_1)} + \frac{e^{-\lambda_2 t}}{(\lambda_1 \cdot \lambda_2)(\lambda_3 \cdot \lambda_2)}$$

$$+ \frac{e^{-\lambda_3 t}}{(\lambda_1 \cdot \lambda_3)(\lambda_2 \cdot \lambda_3)} \right] \cdot \left[\left[U(t) - U(t \cdot \tau)H(t \cdot \tau) \right] \right]$$

$$(2.20)$$

where r is the leach time for a constant leach rate source, and

$$H(x) = \begin{cases} 0 & x < 0 \\ 1 & x \ge 0 \end{cases}$$
 (2.21)

The function U(t) in Equations 2.18 - 2.20 is given by

$$U(t) = \operatorname{erfc}\left[\frac{L_{p} - \frac{v}{R}t}{\sqrt{4\alpha t v/R}}\right] + \exp\left[\frac{L_{p}}{\alpha}\right] \operatorname{erfc}\left[\frac{L_{p} + \frac{v}{R}t}{\sqrt{4\alpha v t/R}}\right], \quad (2.22)$$

where L_p is the total migration path length.

D

The above equations are implemented in NEFTRAN II by defining L_p as the total distanc. from source to discharge (i.e., summing the length of all the legs in the migration path), and v/R as the average isotope velocity (v_{avg}) accounting for retardation. This average isotopic velocity (length/time) is found by preserving the total migration time; i.e.,

$$T_{m} = \frac{\Sigma L_{i}R_{i}}{v_{i}} , \qquad (2.23)$$

where $L_i,\ R_i,$ and v_i are the length, retardation factor and average velocity in the ith leg; thus v_{avc} is

$$v_{avg} = \frac{L_{P}}{T_{m}}$$
 (2.24)

The analytical transport model can only be used to simulate radionuclide transport problems under the following conditions: (1) leach-limited source with a constant leach rate (which is equivalent to the concentration boundary condition given in Table 2.1), (2) chain of three or fewer radionuclides, (3) identical retardation factors for all radionuclides in each leg, and (4) constant fluid velocity. To reiterate, the source used in the analytical transport model is based on the concentration boundary condition given in Table 2.1, and does not utilize the source model contained in NEFTRAN II that is discussed in Section 2.3.

The only remaining point of implementation is the frequency of reporting discharge rates. NEFTRAN II determines a time range for "significant discharge", $T_1 \leq T \leq T_2$, based on the values of T_1 and T_2 given by

$$T_1 = t_M - 4 \sigma_T$$
 (2.25)

and

$$T_2 = T_m + r + 4 \sigma_T$$
 (2.26)

respectively, where σ_T is the standard deviation in time defined by

$$\sigma_{\rm T} = \frac{\sqrt{2 \ \alpha \ L_{\rm p}}}{v_{\rm avg}} \quad . \tag{2.27}$$

 T_1 is small enough to capture the initial breakthrough portion of the discharge curve by subtracting four standard deviations in time from the mean migration time, while T_2 captures the trailing portion of the curve by accounting for the source duration plus the same spread. If the dispersivity is large, it is possible that T_1 is less than the initial source release time. In that case T_1 is replaced by the release time. Similarly, if T_2 exceeds the problem simulation time, it is replaced by the problem simulation time. The resulting time range from T_1 to T_2 is divided by 100 to define a time increment for the analytical transport model, Δt , and discharge is reported 101 times (i.e., $T_1 + i\Delta t$, i = 0, 1,..., 100).

2.3 Source Model

The source model in NEFTRAN II generates source rates for radionuclides exiting the repository and entering a migration path in the geosphere. As discussed above, the analytical transport model incorporates a concentration boundary condition. Therefore, the source model contained in NEFTRAN II is only implemented with the DVM transport model. The source model is executed independently of the DVM radionuclide-transport calculations in NEFTRAN II. Consequently, source rates generated by NEFTRAN II, in principle, could be used in other transport models. Conversely, it would be straightforward (though not currently implemented) to use source rates from other models as input for DVM transport calculations in NEFTRAN II.

The NEFTRAN II source model considers the fraction of the waste inventory in contact with circulating ground water, waste-form leaching, radionuclide solubilities, flow rates, the source area pore volume, and radioactive decay. A fixed delay time for the onset of leaching and/or migration can also be accounted for in the source model. Source model results are cast as time-dependent rates at which each radionuclide enters a migration path. The user provides the initial inventory of radionuclides in the repository as input. The type of radionuclide release scenario being simulated and the extent of the disruption will determine what fraction of the total emplaced waste is accessed by circulating ground water.

Leaching is assumed to be the primary mechanism for the release of radionuclides from the waste form (e.g., glass matrix. The leach rate will depend in part on the matrix material, fluid flow rates and ground-water chemistry. Because NRC contractors other than SNL were charged with developing adequate source term models, NEFTRA'. II only implements two simple leach models. These are a constant lea h rate and an exponential leach rate. In the constant-leach rate model, the amount of waste that leaches per unit time is a constant fraction of the initial mass present. In the exponential model, the amount of waste that leaches per unit time is a constant fraction of the remaining waste mass. The source model was designed so that other leach models can be easily incorporated when available data suggest a need.

Some radionuclides have been shown to be qu te insoluble in ground water due to a low solubility of the radionuclide, a high leach rate from the waste form, and/or a low inflow rate of uncestaminated water. If any of these were the case, there could be more mass of radionuclides free of the waste matrix than can be dissolved in greand water. The NEFTRAN II source model accounts for this phenomenon by maintaining an inventory labeled "leached but undissolved." If such an inventory is necessary, it can act as a source of radionuclides even after all material has been leached from the waste matrix. Solubility limits can, therefore, have the conjunctive effects of lowe ing nuclide concentrations and extending the source pulse in time. Dilution caused by the influx of uncontaminated ground water can reduce contaminant concentrations exiting the repository. Dilution is accounted for by offering an option in NEFTRAN II to treat the repository as a mixing cell; that is, water entering the mixing cell is assumed to instantly, and uniformly, mix with any dissolved material in the cell. The source is then distributed into the transport path based on the diluted concentrations. The oth to option for distributing the source into the transport path in NEFTRAN II is the flow-through source model which distributes the source evenly into the source leg (the first leg in the migration path). The flow-through source model assumes that source material leaves the source volume as it dissolves and dilution by uncontaminated water does not take place.

A new feature in NEFTRAN II allows the flow rate through the repository to change with time. The source model integrates the time-varying flow rate to estimate the total inflow over a time step. Thus, the amount of radionuclide that can dissolve may also change with time. However, this is the only effect of time-varying flow rates since current implementation does not allow the mixing-cell model to be used in conjunction with time-varying flow rates.

As indicated above, there are several different options available in the NEFTRAN II source model. These options can be classified into two different sets. First, there are options related to how the radioactive isotopes become available for transport from the waste form (e.g., leach-limited, solubility-limited, or both). Second, there are options that determine how the repository is to be treated (e.g., mixing-cell source, flow-through source).

Radioactive decay causes the inventory to change with time. The inventory remaining in the waste form (i.e., unleached), the leached-butundissolved inventory, and radionuclide concentrations in water (i.e., dissolved) all decrease due to radioactive decay and potentially increase due to production. These effects are taken into account in the source model contained in NEFTRAN II.

2.3.1 Theory

Before describing the governing equations of the NEFTRAN II source model, the notation used to denote decay chains is discussed. For simplification, it is assumed that species 1 is the parent of species 2 is the parent of species 3, etc. For simplicity this is written as $1 \rightarrow 2 \rightarrow 3$...1. The underlying assumption is that smaller indexed species decay to larger indexed species and that there are no branches in the decay chain. In practice, NEFTRAN II can treat branching using branching fractions supplied by the user. To illustrate the notation, assume that there are I isotopes in a decay chain indexed as described above. The inventory (atoms per mass of waste matrix) for species i is given by

$$\frac{dN_{i}}{dt} = \begin{cases} -\lambda_{i}N_{i} & , \text{ if } i = 1 \\ \\ -\lambda_{i}N_{i} + \lambda_{i-1}N_{i-1} & , \text{ if } 1 < i \le 1 \end{cases}$$

(2.28)

dh

where N_i is the inventory of species i (atoms/mass of waste matrix), λ_i (=ln 2/T_{1/2}) the decay constant for species i (time⁻¹), and T_{1/2} the half-life for species i (time).

Equation 2.28 represent a system of equations that can be solved analytically, and the solutions are known as the Bateman equations. The form of the solution implemented in NEFTRAN II yields decay and production fractions over a time interval from zero to time t. For parent $p \leq 1$ the fraction is given by

$$F_{i}(p,t) = \begin{cases} e^{-\lambda_{i}t} & \text{, if } i = 1 \\ \vdots \\ I \\ j=p \end{cases} \begin{pmatrix} i-1 \\ p \\ j=p \end{cases} \begin{pmatrix} e^{-\lambda_{k}t} & -\lambda_{i}t \\ e \\ \frac{e^{-\lambda_{k}t}}{1} & e^{-\lambda_{i}t} \\ \frac{e^{-\lambda_{k}t}}{1} & e^{-\lambda_{i}t} \\ \frac{e^{-\lambda_{k}t}}{1} & e^{-\lambda_{k}t} \\ \frac{e^{-\lambda_{k}t}}{1} & e^{-\lambda_{k}t}$$

where F_i(p,t) is the fraction of parent p decaying to species i over time t.

The fractions generated by Equation 2.29 can be used to find the emplaced inventory of species i at t by substituting these fractions into

$$N_{i}(t) = \sum_{p=1}^{i} F(p,t) N_{p}(0) , \qquad (2.30)$$

where $N_{c}(0)$ is the initial inventory of species p (atoms/mass of waste matrix),

Equation 2.30 is applied if the user specifies a release time that is greater than zero. This option is useful if one assumes that the waste containers or an engineered barrier in the near-fleid would prohibit farfield transport for a specified period of time.

The governing equation for the rate at which atoms of species i leach from the waste matrix is given by

$$R_{i}(t) = N_{i}(t) \frac{dM(t)}{dt}$$
, (2.31)

where M is the (intact) mass of waste matrix material at time t. If the user selects the constant-leach-rate option, then

$$\frac{dM(t)}{dt} = -\frac{M_0}{T_1} , \qquad (2.32)$$

where $1/T_{\rm L}$ is the leach rate (time $^{-1})$ and $M_{\rm o}$ is the initial waste mass (m).

The solution to Equation 2.32 is

$$M(t) = M_0(1 + t/T_L)$$
 (2.33)

For the exponential-leach-rate option,

$$\frac{\mathrm{dM}(\mathrm{t})}{\mathrm{dt}} = -\frac{\mathrm{M}(\mathrm{t})}{\mathrm{T}_{\mathrm{L}}} \tag{2.34}$$

Solving Equation 2.34 results in

$$M(t) = M_0 e^{-t/T}L$$
 (2.35)

The "leached but undissolved" inventory is described by the following equations

$$\frac{dU_{i}}{dt} = \begin{cases} -\lambda_{i}U_{i} + R_{i} - S_{i} & , \text{ if } i = 1 \\ & & (2.36) \\ -\lambda_{i}U_{i} + \lambda_{i-1}U_{i-1} + R_{i} - S_{i} & , \text{ if } 1 < i \leq 1 \end{cases}$$

where U_i is the leached-but-undissolved inventory of species i (atoms), S_i the rall at which atoms in the leached-but-undissolved inventory enter solution, and R_i is the leach rate given by Equation 2.31.

The formulation for ${\rm S}_i$ depends on the source flow model chosen, flow through or mixing cell, and whether solubilities are treated. Thus,

rather than formulating S_i in this discussion (which NEFTFAN II does not explicitly use) determination of radionuclide concentrations for the two source flow models is discussed in the implementation section (Section 2.3.2). This section is concluded with the theory for the mixing-cell model.

Figure 2.3 illustrates the basic idea of the mixing-cell source model. Water at a certain volumetric flow rate, Q_s (volume time), moves through a constant volume, V_f , and dilutes any dissolved material in the volume. The rate at which dissolved material leaves the mixing cell is

$$S_{(t)} = C(t)Q_{s}(t)$$
, (2.37)

where $S_C(t)$ is the source rate (in mass per unit time) and C(t) the solute concentration (in mass/volume).

The operation of the mixing cell can be illustrated with a simple example. Given a cell of constant pore volume, V_f , with a given flow rate, Q_s , and initial concentration of a dissolved species, C_o , a mass balance shows that the concentration of the species leaving the cell is described by

$$\frac{dC}{dt} = -C \left(\frac{Q_s}{V_f} \right)$$
(2.38)

Integration using the initial condition $C(t=0) = C_{c}$ gives

$$C(t) = C_{o} e^{\left(\frac{Q_{s}t}{V_{f}}\right)}$$
(2.39)

Substituting Equation 2.39 into Equation 2.37 gives

$$S_{c}(t) = C_{o}Q_{s}e^{\left(\frac{Q_{s}t}{V_{f}}\right)}$$
(2.40)

If the user opts, NEFTRAN II will determine whether a mixing-cell-source model is appropriate. The basis for choosing a mixing-cell model is the average particle residence time, T, given by

$$T_r = \frac{v_f}{Q_s} \qquad (2.41)$$



Figure 2.3. The Mixing Cell

If T_r is small compared to the average migration time of an isotope, then it is assumed that all of the material leaves the source volume rapidly, and it is not necessary to use a mixing-cell-source model. Alternatively, if T_r is large compared to the average migration time, there is the possibility of dilution of the source concentration and a mixing cell source is appropriate.

2.3.2 Implementation

The various source model options are all implemented over discrete time steps, Δt_s . The user can specify Δt_s or allow NEFTRAN II to determine an appropriate value. If the user chooses to specify Δt_s , it is strongly recommended that the guidelines implemented in NEFTRAN II to determine Δt_s be followed.

<u>Source Model Time Step Determination</u>. There are four basic criteria used to determine a time step for the source model, these are:

- 1. ensure that the leach pulse is adequately represented,
- 2. ensure that radioactive decay is accounted for accurately,
- ensure that the time step is less than the average residence time in the mixing cell, and
- for the case of time-dependent flow rates through the repository, ensure that the time step is small enough to capture the peak time-dependent flow rate.

The impact of each criterion on Δt_s depends on the source options chosen and the properties of the source region and decay chains. The criteria are defined further by a set of increment-determination parameters. These parameters have default values in the code or can be input directly by the user (see Section 4.3.5). The description that follows is based on the default values.

LEACH PULSE - If leaching is being treated as part of the source model, then at least five time steps across the leach pulse are required.

DECAY - The time step cannot exceed 0.5 times the smallest "important" half-life for all important isotopes. An important isotope is defined as an isotope that has a mean travel time less than the problem simulation time, and a half life and mean velocity such that a significant fraction of its initial inventory will survive decay to discharge. Therefore, an isotope is important if its initial inventory will discharge during the problem time and if the isotope travel time is less than twenty half lives.

RESIDENCE TIME - The user has the option to use a mixing-cell source, a flow-through source or to let the code decide which type of source model is appropriate (see Section 4.3.1). If the mixing cell source is being implemented, then Δt_s cannot exceed 0.2 times the mixing cell residence time, T_r .

FLOW PEAK - For time-dependent flowrates through the repository, $\Delta t_{\rm s}$ should capture the peak time-dependent flow rate. This is done by multiplying a fraction, 0.8, by the peak flow rate. The times greater than and less than the peak flow rate at which this fractional flow rate occurs are determined. These times dictate the time range that bounds $\Delta t_{\rm s}$ to ensure that the peak flow rate is captured. This algorithm may not be sufficient for all time-dependent flow rate profiles.

Leach-Limited Source. If the leach-limited only source option is selected (i.e., solubility limits are not applied), the rate at which a particular radionuclide enters solution, R_i , is given by Equation 2.31. N_i is given by Equations 2.30 and 2.29 and dM/dt is found from either Equation 2.32 or Equation 2.34. If the flow-through source option is selected then R_i is the only information that is needed to determine the source rates for each isotope. In practice, the total amount leached from t to t + Δt_i is found and decay is accounted for by finding the average amount available during this time interval.

If the mixing-cell option is selected, the source concentration for species i must be determined to find the source rate for species i and is given by

$$\frac{dC_{i}}{dt} = \begin{cases} -\lambda_{i} C_{i} + \frac{\lambda_{i}}{V_{f}} - \frac{Q_{s}C_{i}}{V_{f}} & , \text{ if } i = 1 \\ & , \text{ if } i = 1 \\ -\lambda_{i} C_{i} + \lambda_{i-1} C_{i-1} \frac{R_{i}}{V_{f}} - \frac{Q_{s}C_{i}}{V_{f}} & , \text{ if } 1 < i \leq I \end{cases},$$

$$(2.42)$$

where C₁ is the concentration of species i (atoms/volume³).

Equation 2.37 is used to determine the source rates for each isotope, again as averages, from t to $t + \Delta t_{a}$.

<u>Solubility-Limited Source</u>. If the solubility-limited option is selected (i.e., leach-limits are not applied), NEFTRAN II places the entire radionuclide inventory in the leached-but-undissolved inventory at the time of release. Then, for the flow-through-source option, the source concentration (C_i) is given by the minimum of $U_i(t)/(Q_s\Delta t_s)$ or $L_i(t)$, where $L_i(t)$ is the solubility of isotope i (atoms/volume of water).

 C_i is the minimum of the amount that can dissolve without exceeding the solubility limit or the inventory that is left. In other words, as long as there is more mass than can be dissolved, the source rate will be based on the solubility limit of the species. Once the mass is depleted enough to be less than the mass that can dissolve, the source rate will be based on the amount of mass that is left.

If the mixing-cell source option is selected, an intermediate source concentration (\widetilde{C}) is found by accounting for decay, production, and dilution; that is,

$$\frac{d\tilde{c}_{i}}{dt} = \begin{cases} -\lambda_{i} \tilde{c}_{i} + \gamma \tilde{c}_{i} & , \text{ if } i = 1 \\ & & (2.43) \\ -\lambda_{i} \tilde{c}_{i} + \lambda_{i-1} \tilde{c}_{i-1} + \gamma \tilde{c}_{i} & , \text{ if } 1 < i \leq 1 \end{cases},$$

where $\gamma = Q_s/V_f = 1/T_r$ is the dilution factor.

63

.

Solubilities are accounted for by using the equation

$$C_{i}(t) = MIN \left[\overline{C}_{i}(t) + \frac{U_{i}(t)}{V}, L_{i}(t) \right]$$
 (2.44)

<u>Combined Leach and Solubility Limits.</u> The user can elect to apply a leach rate to the waste matrix and solubility limits to radionuclides in solution. In this case, the rate at which radionuclides escape the waste matrix and enter the leached-but-undissolved inventory is given by Equations 2.31 and 2.32 or 2.34, depending on whether a constant leach or an exponential leach rate is being used. The leached-but-undissolved inventory is then found from Equation 2.36.

If the flow-through source option has been selected, the source concentration is given as discussed above for a solubility-limited source. Otherwise, for the mixing-cell source option, the source is determined in two steps, from Equation 2.3 and Equation 2.44.

Apportioning Solubility Limits. In the equations presented above, the solubility limit for species i, $L_i(t)$, was assumed to be time-dependent. However, in practice, solubilities are only available for elements and are constant with time, provided solvent properties are constant. In a typical NEFTRAN II application there may be several isotopes of the same element compating for dissolution. The approach taken in NEFTRAN II is to partition the amount of a particular element that can be dissolved into amounts proportional to the individual isotopes. These isotopes are undergoing radioactive decay/production as time evolves and therefore, their proportions and hence their solubility limits, become time-dependent.

To illustrate the proportioning, suppose element E has isotopes $E_1,\ E_2,\ \ldots,\ E_k.$ The solubility limit for species E_i is given by

$$L_{i}(t) = \frac{U_{i}(t)}{k} \cdot L_{E}$$

$$\sum_{j=1}^{\Sigma} U_{j}(t)$$
(2.45)

where L_g is the solubility limit for element E (atoms/volume).

Thus, the effective solubility limit for species i, L_i , is time-dependent if there are two or more isotopes of element E with different decay or production rates.

<u>Time-Dependent Flow Rates Through the Source</u>. As discussed above, to determine source rates based on solubility limits, the flow rate through the source (repository) is used. The user may provide time-dependent flow rates through the source region from an external file (Section 4.3.1). Although flow rates are also used for the mixing-cell source model, the option to use time-dependent flow rates is currently only available in conjunction with the flow-through source model.

Time-dependent flow rates through the source can also occur if the user provides time-dependent fluid velocities from an external file (Section 4.3.1). In this case, the velocity for the first leg in the migration path is used to determine a time-dependent flow rate through the source. If both options are implemented (i.e., external file of time-dependent flow rates through the source, and an external file of time-dependent fluid flow velocities), the time-dependent flow rates through the source are utilized by the source model.

2.4 Distributed Velocity Method (DVM) Transport Model

The usual run-mode for the NEFTRAN II code implements the DVM transport option. Convective transport is simulated by moving groups or packets of particles (representing dissolved radionuclides) along the flow field over each time step. Dispersion is simulated by allowing the packets to spread simultaneous with convective transport. Thus, DVM is similar to particle tracking methods or the method-of-characteristic. However, what sets DVM apart from these transport simulation methods is the ability to incorporate radioactive decay chains with the direct simulation technique. The following sections describe the theoretical basis of DVM, as well as the numerical implementation of the DVM transport model. The capability unique to NEFTRAN II, DVM transport in time-dependent velocity fields, is also discussed.

2.4.1 Theory

The convective-dispersion transport equation in one dimension can be written as

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} - \overline{v} \frac{\partial \rho}{\partial x} + S , \qquad (2.46)$$

where ρ is the particle density (atoms/volume), \overline{v} is the average particle velocity (length/time) and D is the dispersion coefficient (length²/time). These units of ρ are used because they facilitate the simulation of radioactive decay and can be easily converted to the traditional unit of concentration.

Assuming negligible molecular diffusion, the dispersion coefficient (D) is defined as

$$D = \alpha |v| , \qquad (2.47)$$

where α is the dispersivity (length). In ground-water systems, molecular diffusion is negligible when transport by convection dominates molecular diffusion or, 'f it does not dominate, is the most significant pathway. By defining dispersion coefficient in this manner, NEFTRAN II simulates mechanical dispersion and not hydrodynamic dispersion which includes the effects of molecular diffusion.

When $\rho = 0$ at the infinite boundaries, the solution to Equation 2.46 contains two terms: a particular solution and a complementary solution. Taking the density of particles at time t' to be $\rho(x', t')$, the complementary solution is

$$\rho_{0}(\mathbf{x}, t) = \int_{-\infty}^{\infty} d\mathbf{x}' \rho(\mathbf{x}', t') G(\mathbf{x} - \mathbf{x}', t - t') . \qquad (2.48)$$

the particular solution of Equation 2.46 yields the complete solution

$$\rho(\mathbf{x}, t) = \rho_0(\mathbf{x}, t) + \int_{t'}^{t} dr \int_{\mathbf{x}_0}^{\mathbf{x}_1} d\mathbf{x}' S(\mathbf{x}', r) G(\mathbf{x} - \mathbf{x}', t - r) \quad . \quad (2.49)$$

The Green's function, $G(x\ *\ x',\ t\ *\ t'),$ in Equations 2.48 and 2.49 may be written as

$$G(x + x', t + t') = \frac{1}{\sqrt{2\pi}\sigma_{x}} \exp\left\{-\frac{\left[(x - x') + \overline{v}(t - t')\right]^{2}}{2\sigma_{x}^{2}}\right\}, \quad (2.50)$$
where the variance is

$$\sigma_{\rm X}^2 = 2D(t + t^2)$$
 . (2.51)

G(x - x', t - t') is a spatial Green's function, as indicated by the units of σ_x (i.e., length) and G (i.e., length⁻¹).

Equation 2.50 may be recast as a velocity distribution by considering the illustration in Figure 2.4. This figure shows the evolution of the Green's function over (t - t') from an instantaneous point source function to a Gaussian distribution. Particles arriving at the mean position of this spatial distribution have travelled from x' with velo-

city $\bar{\nu}$. Particles at position x, however, have travelled from x' with an average velocity

$$v = \frac{(x - x')}{(t + t')}$$
(2.52)

If Equation 2.52 is substituted into Equations 2.50 and 2.51 then

$$G(x - x', t - t') = \frac{H(v, t - t')}{(t - t')}$$
 (2.53)

where

$$H(v, t \cdot t') = \frac{1}{\sqrt{2\pi} \sigma_v} \exp\left[-\frac{(v \cdot \bar{v})^2}{2\sigma_v^2}\right] , \qquad (2.54)$$

and

13

$$\sigma_{\rm v} = \int \frac{2D}{(t-t')} = \frac{\sigma_{\rm x}}{(t-t')}$$
 (2.55)

Quantity H is a Green's function in velocity space as indicated by the units of $\sigma_{\rm v}$ (i.e., length/time) and H (i.e., time/length).

Substituting Equation 2.53 into Equation 2.49, gives

$$\rho(\mathbf{x}, t) = \rho_0(\mathbf{x}, t) + \int_{t'}^{t} d\tau \int_{\mathbf{x}_0}^{\mathbf{x}_1} S(\mathbf{x}', \tau) H(\mathbf{v}, t + \tau) / (t - \tau) d\mathbf{x}' \quad (2.56)$$





Recailing Equation 2.52, Equation 2.56 can be written as

$$\rho(\mathbf{x}, \mathbf{t}) = \rho_0(\mathbf{x}, \mathbf{t}) + \int_{\mathbf{t}'}^{\mathbf{t}} dr \int_{\mathbf{v}_0}^{\mathbf{v}_1} S(\mathbf{x}', r) H(\mathbf{v}, \mathbf{t} - r) d\mathbf{v} , \qquad (2.57)$$

where

 $v_{0} = \frac{x + x_{0}}{t + t'}$, (2.58) $v_{1} = \frac{x + x_{1}}{t + t'}$.

and

Thus the transport of an ensemble of particles at position x' and time t' to position x at a later time t can be accomplished by summing over a suitable velocity range weighted by the Green's function in velocity space.

The theoretical basis for DVM is the process of mechanical dispersion which occurs with solute transport through porous media. Specifically, the physical concept embodied in Equation 2.57 is due to heterogeneity of the flow field, a number of alternate paths exist for particles to migrate from x' to x. The underlying assumption is that these paths may be characterized by a continuum of migration times and average velocity components in the direction of flow. By distributing these average velocities according to the Gaussian function developed earlier (Equation 2.54), DVM has been specialized to the conventional Fickian treatment of dispersion. Although there has been some criticism of this conventional Fickian treatment for modeling mechanical dispersion, currently, an alternative does not exist; however, in principle, the DVM technique could be applied to any specified velocity distribution.

2.4.2 Implementation

This section briefly describes the manner in which DVM is numerically implemented. The discussion begins with a single decaying radionuclide. The analysis is then extended to the treatment of a decay chain.

To motivate this discussion of numerical implementation, recall Figure 2.4 which illustrates the movement of an instantaneous point source at position x' and time t' to a Gaussian profile at time t > t' and position x given by x = x' + v (t - t').

In the numerical implementation of DVM, this can be visualized as shown in Figure 2.5. Here, the spatial dimension x is discretized into grid blocks of equal length. The "point source" is confined to a single grid block as shown. However, to model dispersive spreading of the material as it is transported from t' to t, particles in the source block are given a distribution of velocities. As illustrated, particles assigned





to the higher velocity intervals travel farther than those assigned to the lowar velocity intervals. If the velocity intervals are determined from a Gaussian distribution (see Equations 2.54 and 2.55), then the particle density $\rho(\mathbf{x},t)$ approximates a Gaussian distribution in the spatial dimension.

So, for the *l*th leg having mean fluid velocity, \overline{v}_{fl} (length/time) and dispersivity a_{l} (length), velocities for *t*he jth velocity interval, v(l,r,j), are found for species r as follow:

$$\mathbf{v}(\ell,\mathbf{r},\mathbf{j}) = \mathbf{r}_{\mathbf{j}} \left[\frac{2\alpha_{\ell} \overline{\mathbf{v}}_{\mathbf{f}\ell}}{\Delta t \mathbf{R}_{\ell}} + \frac{\overline{\mathbf{v}}_{\mathbf{f}\ell}}{\mathbf{R}_{\ell}} \right], \qquad (2.59)$$

where R is the retardation factor (dimensionless) for species r in the lth leg, and c is the jth abcissa from a standard normal distribution given by

$$\frac{2j-1}{2N_{v}} = \int_{-\infty}^{\varepsilon} j \frac{1}{\sqrt{2\pi}} e^{-0.5u^2} du, j = 1, \dots, N_{v}, \quad (2.60)$$

where N_v is the number of velocity intervals.

For clarity, Figure 2.5 presents the DVM transport, as applied to a single source block at time t' and the several resulting receiver blocks at time t > t'. In actual application, however, it is numerically more efficient to determine the contributions to a single receiver block at time t from multiple source blocks at time t' < t. This approach is discussed in the following sections.

One Decaying Radionuclide. Here, only the propagation of the density function $\rho(\mathbf{x}', \mathbf{t}')$ from time t' to time t (Equation 2.57) is considered. There are $N_{\mathbf{x}}$ equal-space increments of length $\Delta \mathbf{x}$ and the time increment $\Delta \mathbf{t}$ is taken to be constant. The velocity dimension is divided into $N_{\mathbf{v}}$ increments based on equal probability. While DVM can be generalized to variable spatial and time increments, such generalization is not considered in NEFTRAN II as will become clear in the discussion that follows.

Propagation of densities over Δt for velocity subgroup j m is written as

$$\Delta \rho(i, j, t) = D_{f} W(j) \left\{ M_{f}(j) \rho \left(1 - k_{j}, t' \right) \right.$$

$$\left. + \left[1 - M_{f}(j) \right] \rho \left[1 - k_{j} - 1, t' \right] \right\} .$$
(2.61)

Although the argument list in Equation 2.61 appears formidable, it can be readily understood. As indicated there, the contribution to receiver block i for velocity interval j is determined by three fractions: a geometric mixing fraction, M_f , a velocity-interval fraction, W, and a decay fraction, D_f .

 M_f may be understood by referring to Figure 2.6. Looking at velocity interval j, one sees that there are, in general, two contributions to receiver block i. One is a packet of particles coming from donor block i - k and the other is a packet of particles coming from donor block i - k - 1. Although not intuitively obvious, the reason there are only two contributions is because the physical dimension of a packet of particles is the actual grid block size. As is also indicated in Figure 2.5, there is generally only partial overlap of the propagated block contents with receiver block i. The donor block index k, is

$$k_{j} = \left[\left[\frac{v_{j} \Delta t}{\Delta x} \right] \right] , \qquad (2.62)$$

where [z] is the greatest integer $\leq z$,

and v_{1} is determined from

$$\left(\frac{j-\frac{1}{2}}{N_{v}}\right) = \frac{1}{\sqrt{2\pi}\sigma_{v}} \int_{-\infty}^{v_{j}} \exp\left(-\frac{\left(v-\frac{1}{v}\right)^{2}}{2\sigma_{v}^{2}}\right) dv \quad (2.63)$$

The corresponding mixing fraction is

$$M_{f}(j) = 1 \cdot \left[\frac{v_{j} \Delta t}{\Delta x} \cdot k_{j} \right] . \qquad (2.64)$$



2

Figure 2.6. Illustration of the Mixing Fraction Concept

Because the velocity dimension is divided into intervals assuming equal probability, the weight W(j) assigned the jth velocity interval is

$$W(j) = \frac{1}{N_v}$$
 (2.65)

The decay fraction is taken to be

$$D_{f} = e^{-\lambda\Delta t} \quad . \tag{2.66}$$

With these three fractions defined, Equation 2.61 is summed over all velocity intervals to obtain the total particle density in grid block i:

$$\rho(1,t) = \frac{D_{f}}{N_{v}} \sum_{j=1}^{N_{v}} \left\{ M_{f}(j) \ \rho(1 - k_{j}, t') + (1 - M_{f}(j)) \right\}$$

$$\rho(1 - k_{j} - 1, t') \left\}$$

$$(2.67)$$

As a last step in this discussion, Equation 2.67 is rewritten in a more computationally efficient form. To do this, the possibility of deg eracy with respect to the index $k_{\rm j}$ is addressed. This degeneracy could mean either

$$k_{j+1} = k_j$$
 or $k_{j+1} = k_j + 1$. (2.68)

Taking such degeneracies into account yields the expression

$$\rho(i,t) = \sum_{j=1}^{N_B(i)} B(j) \rho\left(i - k_j, t'\right) . \qquad (2.69)$$

Quantities $N_B(i)$ and B(j) are most easily obtained by a computational procedur, which makes the tests of Equation 2.68 and accumulates the coefficients to form the matrix of B.

portant to note that, as long as Δx and Δt are constants, B is a sector which contains at most 2 \cdot N_v terms. Furthermore, B(j) may puted during the initial setup before the actual transport simulation is conducted. For unequal grid block increments Δx , B would be

dependent on grid block index 1, and for unequal time increments Δt , B would have to be re-evaluated for each change in time increment. Thus, it is most efficient to maintain fixed Δx and Δt .

The implementation just described corresponds to DvM as it was implemented into the NWFT/DVM code (Campbell, and others, 1981a, 1981b). The same implementation exists in NEFTRAN (Longsine, and others, 1987) and in NEFTRAN II. However, in the latter two codes, the restrictions of constant Δx and Δt were relaxed. In NWFT/DVM, the legs along the migration path were combined into a single leg with each isotope assigned an average velocity over that leg which preserved total mean migration time. This leg-averaged path option is still in NEFTRAN and NEFTRAN II, bowever, with the addition of the matrix diffusion capability to NEFTRAN, it became necessary to treat each leg individually. This treatment was necessary since the residence time in a leg characterized by dual porosity is one of the primary factors that determines the amount of diffusion. The implementation in NEFTRAN and NEFTRAN II is to treat each leg as a distinct unit with (1) a fixed space step for the leg and transport of particles in the interior of the leg described by the B array above, (2) allowing the space step to be different for each leg along the migration path, and (3) computing the fractions of grid blocks in one leg that contribute to blocks in another leg over a time step as a separate model. Thus, a new model, referred to as the leg-to-leg transfer model, was implemented as described in Section 2.4.9.

NEFTRAN II relaxes the fixed time-step restriction. NEFTRAN II simulates time-dependent flow fields by approximating the changing velocities with a step function (see Section 2.4.11). In particular, the user defines time intervals over which the fluid velocity is relatively constant and sequences these intervals from release time to the end of simulation. Over each of these time intervals, a time step is chosen and implementation occurs as described above. However, because the intervals can be of different length and with the changing fluid velocities, it is likely that accuracy and efficiency considerations will dictate the use of a different time step for each time interval. Thus, following each time interval, the code recomputes the transport fractions based on the new velocities and new time steps to be used for the next time interval.

<u>A Chain of Radionuclides</u>. Here the starting point is similar to Equation 2.61, and for species r of a radioactive decay chain it may be written as follows

$$\begin{split} \Delta \rho(\mathbf{i}, \mathbf{j}, \mathbf{r}, \mathbf{r} + \mathbf{p}, \mathbf{t}) &= \mathsf{D}_{\mathbf{f}}(\mathbf{r}, \mathbf{r} + \mathbf{p}) \mathbb{U}(\mathbf{j}) & \bullet \\ & \left\{ \mathsf{M}_{\mathbf{f}}(\mathbf{j}, \mathbf{r}, \mathbf{r} + \mathbf{p}) \bar{\rho} \Big[\mathbf{i} - \mathbf{k}_{\mathbf{j}}, \mathbf{r} - \mathbf{p}, \mathbf{t}' \Big] \\ &+ (\mathbf{1} - \mathsf{M}_{\mathbf{f}}(\mathbf{j}, \mathbf{r}, \mathbf{r} - \mathbf{p})] & \bullet \\ & \rho \Big[\mathbf{i} - \mathbf{k}_{\mathbf{j}} - \mathbf{1}, \mathbf{r} + \mathbf{p}, \mathbf{t}' \Big] \Big\} . \end{split}$$
(2.70)

In this equation Δp is the incremental particle density for isotope r, grid block i, velocity subgroup j, and time t which arises from decay of isotope r - p over time interval t - t'. If p = 0, Equation 2.70 simplifies to Equation 2.61.

 M_f , the mixing fraction, is determined by Equations 2.62 and 2.64 as before. The only difference is the velocity. Because of sorption effects, the velocity will, in general, change with species during the decay $r - p \rightarrow r - p + 1 \dots \rightarrow r$ which occurs during time step Δt . Hence, in this case, the velocity v (j, r, r - p) represents a species average over the time interval $\Delta t = t - t'$. The model used in NEFTRAN II to determine these species average velocities is presented in Section 2.4.6. W, the velocity subgroup fraction, is taken from Equation 2.65 as before.

The role of quantity D_f in Equation 2.70 is expanded beyond that in Equation 2.61. In Equation 2.61, D_f denotes that fraction which survives decay during Δt . In Equation 2.70, D_f pertains to decay only when p = 0, i.e.,

$$D_{r}(r, r - \gamma) = e^{-\lambda \Delta t}, \quad p = 0$$
, (2.71)

Otherwise, this quantity denotes production of species r from species r - p, and may be developed from the Bateman equations (see Section 2.3.1) as

$$D_{f}(r, r - p) = \prod_{q=1}^{p} \lambda_{r-q} \sum_{i=1}^{p} \frac{e^{-\lambda_{r-i}\Delta t}}{\prod_{q=1}^{p} \left(\lambda_{r-j} - \lambda_{r-i}\right)}, \quad p \neq 0 \quad . \quad (2.72)$$

$$j \neq 0 \quad j \neq i$$

This equation, when coupled with appropriate mixing and weighting functions, may be viewed as a model for evaluating that portion of the source integral in Equation 2.57 which is appropriate for radioactive decay processes.

To complete the analysis of radioactive decay chains, Equation 2.70 is summed over all velocity subgroups j and all parents p of species r. This yields

$$\begin{split} \rho(i, r, t) &= \sum_{p=0}^{N} \sum_{j=1}^{N_v} D_f(r, r + p) W(j) \bigg\{ M_f(j, r, r + p) \\ &= \rho \Big(i + k_j, r + p, t' \Big) + [1 + M_f(j, r, r + p)] + (2.73) \\ &= \rho \Big(i + k_j + 1, r + p, t' \Big) \bigg\} \,. \end{split}$$

2-32

Rocollecting the sum then gives the working equation

$$\rho(i, r, t) = \sum_{p=0}^{N_{p}(r)} \sum_{\substack{j=1 \\ j=1}}^{N_{B}(i, r, r + p)} \Psi(j, r, r + p) \Psi(i, k_{j}, r + p, t'). \qquad (2.74)$$

The upper bounds in Equation 2.74 are expressed as functions. The dependence $N_p(r)$ reflects the fact that, in general, each radionuclide has a different number of parents. Furthermore, one may want to arbitrarily impose a bound on the parint sum. The limit $N_p(i, r, r, r)$ gives the number of grid blocks which contribute to a receiver block i. The limit carries radionuclide indices because of the transport velocity model (Section 2.4.6). As in the case of a single decaying nuclide, B will not vary with grid block or time step indices provided that Δx and Δt do not vary. Thus the B matrix may be generated during the setup process. For each r, the B matrix can be viewed as $N_p(r) + 1$ separate vectors each having dimension less than or equal to $2 \cdot N_p$. Hence, computer storage is not a problem. For purposes of comparison with other numerical techniques, Equation 2.74 is an <u>explicit</u> relation in that each term on the right-hand side is known prior to solution for the unknown density p(i, r, t).

The implementation of DVM over a given time interval requires a fixed space step for each leg and a fixed time step for the time interval. The user can specify the space and/or time steps or allow NEFTRAN II to determine appropriate values. If the user chooses to specify the space and/or time steps, it is strongly recommended that the guidelines implemented in NEFTRAN II to determine Δx and Δt be followed. For this reason, the next two sections discuss the guidelines in detail. The discussion follows the code logic which first finds the time step and then the space step(s).

2.5.3 Time Step Determination

The three basic criteria used to determine a time step for transport are:

- ensure that packets cannot jump from source to discharge (for the path-overaged simulations) or skip a leg (for leg-to-leg simulations) in a single time step,
- ensure that there are adequate points to resolve the breakthrough portion of the discharge curves (for path-averaged simulations only), and
- require a minimum nominal number of time steps for the simulation.

The extent to which each of the criteria restricts the size of *i*t depends on the migration time, dispersivity, and half-lives modeled. The criteria are defined further by a set of increment-determination parameters. These parameters have default values in the code or can be input by the user (see Section 0.3.5). The description that follows is based on the default values that are appropriate for the repeated runs involved in statistical Monte Carlo simulations.

Avoid Leg Jump. The time step at is initialized to the minimum travel time which is defined as:

$$T_{\min} = \frac{L_p}{v_{\max}}$$
(2.75)

for the path-averaged case or

$$T_{\min} = MIN \left\{ \frac{Z_{i}}{\frac{1}{\sqrt{max}}} \right\}$$
(2.76)

for the leg-to-leg transfer case. $L_{\rm p}$ is the total migration path length and $Z_{\rm j}$ is the length of leg i. For the leg-to-leg transfer case, the minimum is taken over all legs i and for both definitions, $v_{\rm max}$ (length/time), is the maximum distributed isotope velocity in the path or leg.

 v_{max} is found based on the normal distribution of 12otope velocities (see Section 2.4.2). This is done by approximating the normal distribution of velocities to find the velocity of the last and therefore, largest velocity interval.

Since v_{max} depends on Δt (more precisely, the inverse square root of Δt), the relations

$$v_{max} \Delta t \leq L_p$$
, (2.77)

and

$$v_{\max} \Delta t \leq Z_i$$
 (2.78)

can be transformed into quadratic relations in Δt . These quadratic forms are solved in NEFTRAN II to get an initial value for Δt .

<u>Curve Resolution</u>. The curve-resolution restrictions for Δt are implemented only for the path-averaged case. This criterion is based on finding the standard deviation in the of the breakthrough curve and setting Δt equal to one standard deviation. This ensures that rates are output on the breakthrough portion of the discharge curve. This criterion is only applied for important isotopes. The definition of a important

isotope is similar to the one discussed in conjunction with the source time step in Section 2.3.2. However, for transport, an isotope is considered important if its average migration time is less than the problem simulation time, and if the average migration time is less than 10 times its half-life, compared to 20 times its half-life for source calculations.

After the minimum (over important isotopes) standard deviation is found, a criterion is applied that does not allow T_{min} to be decreased by more than a factor of 0.2.

Nominal Number of Time Steps. This criterion requires a minimum of 30 time steps for a simulation time, or for the time-dependent velocity case, for a time interval. This criterion is needed since it is possible that the first two criteria resulted in a time step that exceeds the problem simulation time.

2.4.4 Spatial-Step Determination

Following the time-step determination, NEFTRAN II finds the spatial gridding. The three criteria used in determining the spatial step are:

- ensure a nominal number of grid blocks in each leg or the entire transport path,
- ensure that Courant numbers are bounded from below for important isotopes, and

The extent to which each of the criteria restricts the size of Δx depends on the migration time, half-lives of the isotopes being modeled, and the time step. The criteria are defined further by a set of incrementdetermination parameters. These parameters have default values in the code or can be input by the user (see Section 4.3.5). The description that follows is based on the default values for these parameters.

Nominal Number of Blocks. The number of grid blocks for a path-averaged simulation is initialized to 50 meaning Δx is initialized to Lp/50. Similarly, for a leg-to-leg transfer problem, the space step for leg i is initialized to $\Delta x_i = z_i/7$, where z_i is the length of leg i. The next two criteria can only reduce or maintain these values for Δx , they will not increase them.

<u>Courant Numbers</u>. This criterion is based on the Courant number and is concerned with the numerical accuracy of NEFTRAN II. As discussed by Campbell and Longsine (1981), for the DVM transport model, numerical dispersion can be controlled by the mcgnitude of the Courant number. The Courant number is defined as In general, to minimize numerical dispersion for the DVM transport model, CN should be greater than or equal to 1.0 for all important isotopes.

Since Δt and ν are known, the CN is set to 1.5 and Δx is determined. This applies to both path-averaged and leg-to-leg transfer cas .

Source Length. For the path-averaged case, and if a flow-through source is being used, Δx is constrained by the length of the source leg. Specifically, the space step cannot be greater than the length of the first leg since this determines the source blocks for the flow-through source model.

At this point, the largest permissible time step and spatial gridding have been selected within the constraints of the problem, based on the increment-determination parameters. Large values reduce computer execution time, which is desirable especially for statistical Monte Carlo simulations. In addition, large time stops also promote accuracy by limiting numerical dispersion This is evident from the Courant number criterion above and is discussed in detail by Campbell and Longsine (1981). The apparent excessive attention to accuracy that is evident in the velocity model (Section 2.4.6), the discharge model (Section 2.4.7), the distribution of source into grid blocks (Section 2.4.5), and the legto-leg transfer model (Section 2.4.9) is required because of the large time steps that are used to limit numerical dispersion. For runs in which discharge of short-lived isotopes must be characterized, time steps should probably be smaller than that which is determined with the criteria discussed above and in Section 2.4.3. The reader is referred to Section 4.3.5 for suggestions to make the space- and time-step selection process more restrictive.

For simulations with steady-state velocity fields, the space and time steps found above are used throughout the entire problem simulation time. For simulations involving time-dependent velocity fields, a new space and time step are selected for each time interval as described above. An appropriate time step for each time interval is determined and stored. Space steps are found for each leg and the smallest space step is retained. Thus, the spatial gridding does not change from time interval to time interval. For all problem types, NEFTRAN II performs dimension checks for the number of grid blocks versus the size of arrays that contain atoms per grid block per isotope. If dimensions are exceeded, either Δx 's are increased and a warning message is written or the code aborts the run, depending on the severity of the excess.

2.4.5 Courant Numbers and Isotope Travel Times

The purpose of this section is to explain the importance of CN and isotope travel time when simulating radionuclide transport with NEFTRAN II. With numerical transport models using finite-difference (FD) or finite-

element (FE) methods, the accuracy of the transport simulation increases with decreasing time step. Thus, one can always improve accuracy with FD- or FE-based codes (at the expense of increased computer time) by simply decreasing the size of the time step. However, with DVM, numerical accuracy is generally improved by increasing the size of the time step. The reasons for this counter intuitive situation are explained by Campbell and Longsine (1981) and are not discussed here. The Sact that DVM likes a large time step has the obvious benefit of reducing computer time (by factors of 10 or more over FD- and FE-based codes). However, this also implies that there is no trivial rule of thumb (such as decreasing the time step for FD or FE) for improving accuracy. The user should have the largest time step possible consistent with considerations of the time dependence of the source rate, isotope half lives, and desired resolution of the breg'through curve. Because of the difficulty of finding the "optimum" space and time step for a given calculation. NEFTRAN II will automatically select a space and time step if the user simply enters zeroes for these values.

NEFTRAN II will usually do an adequate job of selecting a space step and time step. However, the user should generally print out space and time step information, as well as velocity model and retardation information in order to assure that reasonable numerical criteria are being met. The most important indicator of the numerical accuracy of NEFTRAN II is the CN.

The general rule concerning the CN is that it should be greater than or equal to one for all important isotopes. As discussed in previous sections, an important isotope is one that is expected to d'scharge from its initial inventory during the problem simulation time. Conversely, an unimportant isotope is one that is not expected to discharge in significent amounts from its initial inventory during this time. In NEFTRAN II, for DVM transport, an unimportant isotope is one with travel time significantly larger than the problem simulation time or one with a half life less than one-tenth of the travel time. In the first case, the isotope will not discharge from its initial inventory because it will not reach the discharge point during the problem simulation time. In the second case, the isotope will decay to insignificantly low concentrations before discharging.

It is useful to examine the effects of CN on numerical accuracy using NEFTRAN II. Figure 2.7 compares breakthrough curves generated using NEFTRAN II (DVM option) with an analytical solution. The travel time in this example is 500 years. The analytical solution is shown as a solid curve. NEFTRAN II results are shown for CN = 0.1, 1, and 2. For CN = 0.1, substantial numerical dispersion is apparent, while for CN = 1, the numerical dispersion is practically insignificant. The curve for CN = 2 is indistinguishable from the analytical solution. If the user is interested in the integrated discharge at 1000 years or the concentration (or dose) at any time after about 700 years, any of the three DVM curves would probably be adequate. However, suppose the user is interested in the concentration at 400 years. In this case, the most accurate curve between CN = 1 and CN = 2 would be used. To emphasize this point,



----- DVM. CN - 1.0

..... DVM, CN = 2.0



consider Figure 2.8 which presents the same results as Figure 2.7 but with concentration plotted on a logarithmic scale. At 400 years, the concentration predicted using DVM with CN = 2 matches the analytical solution very well. For CN = 1, at 400 years, DVM overestimates the concentration predicted by the analytical solution by about a factor of 2, while for CN = 0.1, the over prediction is as much as three orders of magnitude. The message is that if concentration (or dose, etc.) at some time less than the travel time (when the discharge is greater than zero only because of physical dispersion) is the quantity of interest, it is very important that CN > 1. At later times, the values of CN is less critical, but should still always be greater than or equal to 1 for all important isotopes.

Figure 2.9 is included to help keep the above discussion in perspective. In this figure, the same analytical solution is compared to results generated using a finite difference transport code. The FD case with $\Delta x = 20$ and $\Delta t = 1$ shows about the same level of accuracy (or inaccuracy) as the earlier DVM case with CN = 0.1. The FD case in Figure 2.9 with $\Delta x = 1$ and $\Delta t = 0.5$ shows about the same accuracy as DVM with CN = 1. However, the FD calculation took about 15 minutes compared to a few seconds with NEFTRAN II. No attempt was made with the FD code to generate results as accurate as the DVM case with CN = 2.

It should be apparent from the above discussion that the NEFTRAN II user not only needs to be aware of the value of CN, but also the travel time in a given transport calculation. Before discussing travel time considerations, a few definitions are necessary.

The nominal or average isotope travel time is defined as:

$$T_{D} = \frac{L}{v}$$

where T_n is the average isotope travel time, v the average isotope velocity (ground-water velocity divided by isotope retardation factor in units of length/time), and L the path length from the source to the discharge point.

In attempting to determine whether an isotope will discharge during the problem simulation time, one could compare T_n with the problem simulation time. However, because of dispersion, discharge of an isotopa begins some time before its average travel time. Thus, some approximation of the time of first isotope breakthrough is needed. To estimate this time, consider that the shape of the breakthrough curve near the average travel time is approximately that of an error function (i.e., the integral of a normal distribution). The standard deviation in time underlying the breakthrough curve can be estimated as

$$\alpha_{\rm T} = \sqrt{\frac{2\alpha L}{v}} , \qquad (2.81)$$

(2.80)









where α_T is the standard deviation in time, α the dispersivity (length), L is the migration path length, and v the average isotope velocity (length/time). The minimum travel time or the approximate time to first breakthrough is estimated as

$$T_{e} : T_{n} - Ma_{T}$$
, (2.82)

where T_m is the approximate time to first breakthrough, T_n the average isotope travel time, and M some multiplier to be determined.

Experience indicates that M = 2.3 gives a good approximation to the time of first isotope breakthrough. The next example should help clarify the above ideas on travel time and isotope breakthrough.

For this example, consider the decay chain

The path length is 1000 feet, the dispersivity is 40 feet, and the fluid velocity is 0.1 ft/year. The retardations, average isotope velocities, average isotope travel times, standard deviation in time, and approximate time to first breakthrough are given in Table 2.2.

Table 2.2

Parameters for Example Problem

ISOTOPE	RETARD.	v	T_n	$\alpha_{\tilde{1}}$	T _m
Am243	150	6.67E-4	1.50E6	4.24E5	5.25E5
Pu239	15	6.67E-3	1.50E5	4.24E4	5.25E4
U235	75	1.33E-3	7,50E5	2.12E5	2.62E5

If $T_m > TUB$, the isotope is not expected to discharge in significant amounts and is thus classified as "unimportant." For illustration, the example problem was run for problem times TUB of 1.0 x 10⁵, 5.0 x 10⁵ and 1.0 x 10⁶ years. For TUB = 1.0 x 10⁵ years only ²³⁹Pu should be considered important because T_m for both ²⁴³Am and ²³⁵U are greater than TUB. For ²³⁹Pu, CN = 1.35, while for ²⁴³Am and ²³⁵U, CN < 1. It is obvious that NEFTRAN II focused its space and time step considerations on ²³⁹Pu as the travel times for the other two isotopes are too long to reach the discharge point during the problem simulation time. Figure 2.10 shows discharge rates for this case. As expected, ²³⁹Pu begins to discharge at about 50000 years. However, ²³⁵U also shows some discharge. This occurs



Figure 2.10. Discharge Rate Curves for Problem Simulation Time = 1.0 x $10^5 \ y$

because ²³⁹Pu decays along the migration path to ²³⁵U, some of which is then able to reach the discharge point. None of the original source of ²³⁵U reaches the discharge point in this calculation.

The CN for TUB = 5.0 x 10⁵ years are 6.8 for ²³⁹Pu, 4.3 for ²³⁵U and less than 1 (0.6) for ²⁴³Am. By referring to Table 2.2, it is evident that both ²³⁹Pu and ²³⁵U are expected to travel from the source to the discharge point during the problem time. Consequently, NEFTRAN II has increased the size of the time step so that both isotopes have CN > 1. However, NEFTRAN II did not try to satisfy CN > 1 for ²⁴³Am which has a minimum travel time slightly greater than 500000 years. Discharge curves for this case are shown in Figure 2.11. ²³⁹Pu again breaks through at approximately the expected time, while ²³⁵U produced by decay of ²³⁹Pu begins discharging at approximately this time also. Note that at approximately 2.5 x 10⁵ years, ²³⁵U discharge begins to increase. This corresponds to arrival of the original source inventory of ²³⁵U.

CN for TUB = 1.0 x 10⁶ years for all three isotopes are > 1. The discharge rate curves for TUB = 1.0 x 10⁶ years are shown in Figure 2.12. Note than ²⁴³Am does not discharge in 1.0 x 10⁶ years even though its minimum travel time is about 5.0 x 10⁵ years. The reason is that the half-life of ²⁴⁵Am is only 7.37 x 10³ years so that all the initial inventory for this isotope has decayed before it reaches the discharge point. The reason that ²⁴³Am was apparently considered important (i.e., CN > 1) is that NEFTRAN II was able to produce CN > 1 for the important isotopes (²³⁰Pu and ²³⁵U) and meet other numerical criteria by simply using the default minimum number of time steps (i.e., the default maximum time step size). This default time step just happened to be large enough to give CN > 1 for ²⁴³Am.

It is not a ways possible for NEFTRAN II to achieve CN > 1 for all important isotopes. In the above example, the retardation factors, and hence, the isctope velocities, vary one order of magnitude. Consequently, the largest CN is a factor of 10 larger than the smallest. Suppose the velocities varied over three orders of magnitude. If the slowest isotope were "important" (i.e., expected to discharge) and NEFTRAN II were to select Δx and Δt such that this isotope had CN > 1. then the fastest isotope would have CN > 1000. That is, the fastest isotope would jump 1000 grid blocks each time step. The time step is limited such that the migration path cannot be traversed in one time step and, therefore, to obtain a CN > 1000, more than 1000 grid blocks would be required. For NEFTRAN II, the dimensions are limited to 1000 grid blocks and it would not be possible to satisfy CN > 1 for the important isotope in this example without exceeding dimensions. A compromise Δx and Δt would have to be selected or the dimensions increased. Alternatively, should such a case occur in practice, the user may want to appeal to the physics of the problem. For example, could the very slow moving isotope be left in the source calculation to affect solubilities but not transported? If the isotope is at the bottom of a chain, can it be simply ignored or just take on the Courant number of its parent if it would only discharge with its parent isotope? Another alternative might be to break the decay chain at the slow moving isotope if it is sufficiently long-lived.



Figure 2.11. Discharge Rate Curves for Problem Simulation Time = 5.0 \times $10^5~\rm{y}$





In summary, to get accurate discharge rate results using NEFTRAN II, the user must be aware of isotope travel times, half lives, and CN. In general, CN for important isotopes should be > 1. Important isotopes are those with half lives sufficiently long (> 10% of the minimum travel time) and velocities sufficiently large (minimum travel time < problem simulation time) that they are expected to discharge from their initial inventory during the problem simulation time. In most cases, it is probably not necessary to estimate a minimum travel time but simply to examine the isotope velocities provided by an optional NEFTRAN II output file. As a final summary point, the user must recognize the inherent difficulty in trying to transport chains that have a very large range of velocities. In this case, Courant numbers for the slowest isotopes may have to be compromised. In most realistic cases, however, these isotopes will have such long travel times that they will be classified as unimportant.

2.4.6 Species Velocity Model

As indicated in Section 2.4.2, application of the DVM transport model to a radioactive decay chain requires a method for determining the average velocity of atoms that decay to daughter products during a time step, Δt . As an example, consider the simple decay chain

 $A \rightarrow B$

and suppose that A and B have different retardation factors and therefore, different average velocities. To transport all the atoms in a particula grid block, it is necessary to separately transport those A atoms cha. survive decay during Δt , atoms of isotope A that decay to B during Δt , and finally, atoms of isotope B that survive decay during Δt . That is, one must transport 3 "subchains" namely.

A		A	velocity	VA
A	-5	В	velocity	VAR
В	-*	В	velocity	VB

As velocities v_A and v_B are assumed known, the problem is to calculate v_{AB} , the average velocity for atoms of isotope A that decay to B (and remain as B to Δt) during Δt . One can write v_{AB} as

$$\mathbf{v} = \mathbf{\overline{T}} + \mathbf{v} + \begin{bmatrix} \Delta \mathbf{t} + \mathbf{\overline{T}} \end{bmatrix} \mathbf{v}$$

$$\mathbf{AB} = \mathbf{A} + \mathbf{A} \begin{bmatrix} \Delta \mathbf{t} + \mathbf{\overline{T}} \end{bmatrix} \mathbf{v}$$

$$\mathbf{B} = \begin{bmatrix} \mathbf{t} & \mathbf{t} \\ \mathbf{t} & \mathbf{t} \end{bmatrix} \mathbf{E}$$

$$(2.83)$$

where T_A is the average time spent as A for atoms that decay to B during Δt . T_A is found by writing the probability that, in time interval Δt , species A decays to B which survives to the end of Δt . This probability is written as:

$$DP(A \rightarrow B) = \begin{pmatrix} \lambda_A t \\ e \end{pmatrix} \begin{pmatrix} \lambda_A dt \end{pmatrix} \begin{pmatrix} \lambda_B (\Delta t - t) \\ e \end{pmatrix}$$
 (2.84)

The first term in parentheses is the probability that species A survives to time t. The second term is the probability that A decays to B during infinitesimal time dt. The last term is the probability that B survives decay to the end of Δt . Thus, the probability that species A decays to species B over Δt is an integral of the product of independent probabili-

ties. To find $\overline{T}_A,$ the integrand is weighted by t and the resulting integral is divided by DF(A+B). This is equivalent to

$$\widetilde{T}_{A} = \frac{\int_{0}^{\Delta t} t_{\lambda_{A}} e^{-\lambda_{A}t} e^{-\lambda_{B}(\Delta t + t)} dt}{\int_{0}^{\Delta t} \frac{\lambda_{A}t}{\lambda_{A}} e^{-\lambda_{B}(\Delta t + t)} dt}$$
(2.85)

The solution of Equation 2.85 is

$$\overline{T}_{A} = \frac{e^{(\lambda_{b} + \lambda_{a})\Delta t}}{e^{(\lambda_{b} + \lambda_{a})\Delta t}} \Delta t - \frac{1}{\lambda_{b} + \lambda_{a}}$$
(2.86)

Substitution of Equation 2.86 into 2.83 yields $v_{AB}.$ This approach is extended to decay chains of several isotopes in Appendix A.

The implementation of DVM is based on the transport of subchains within a given decay chain. For example, suppose the decay chain $I_1 \rightarrow I_2 \dots \rightarrow I_5$ is to be transported. In DVM, 15 subchains are potentially transported over each Δt . These subchains are

I ₁	$\mathbb{I}_1 {\rightarrow} \mathbb{I}_2$	$I_1 \rightarrow I_2 \rightarrow I_3$	$\mathbb{I}_1 {\xrightarrow{\scriptstyle \rightarrow}} \mathbb{I}_2 {\xrightarrow{\scriptstyle \rightarrow}} \mathbb{I}_3 {\xrightarrow{\scriptstyle \rightarrow}} \mathbb{I}_k$	$\mathtt{I}_1 {\rightarrow} \mathtt{I}_2 {\rightarrow} \mathtt{I}_3 {\rightarrow} \mathtt{I}_4 {\rightarrow} \mathtt{I}_5$
	I 2	I₂→I₃	$\mathbb{I}_2 {}^{\rightarrow} \mathbb{I}_3 {}^{\rightarrow} \mathbb{I}_4$	$\mathbb{I}_2 {}^{\rightarrow} \mathbb{I}_3 {}^{\rightarrow} \mathbb{I}_4 {}^{\rightarrow} \mathbb{I}_5$
		I3	I ₃ →I ₄	I3-I4-I5
			1.	I4→IS
				I_5

Column 4, for example, includes the subchains necessary to update the amounts and locations of species I_4 . However, the contribution to species I_4 over a single time step from species I_1 and (possibly) species I_2 may be insignificant due to the relative half-lives of each species. If this is the case, it is reasonable to transport only $I_3 \rightarrow I_4$ and I_4 . Past experience indicates that restricting subchains to a maximum length of five is adequate. Encountering the need to transport a six-member subchain is not anticipated and, in fact, has never been noted. However, when subchains of length 6 or greater are encountered, an approximate scheme, presented in Appendix A, is used.

2.4.7 Discharge Model

Determining total discharge of species r from t to t + Δt is based on evaluation of

$$\delta(r, t, \Delta t) = \sum_{p=0}^{q} \sum_{i=1}^{NB(r, r-p)} F(r, r-p, i) \rho(r-p, N_x - i + 1, t) , \qquad (2.87)$$

where NB(r, r - p) marks the grid block farthest from the boundary that contains precursor r - p and can contribute to the discharge of r, F(r, r - p,i) is the fraction of species r - p in grid block N_x - i + 1 that discharges as species r, and $\rho(r - p, N_x - i + 1, t)$ is the number of atoms of species r - p in grid block N_x - i + 1 at time t.

The determination of array F (and as a by-product, the array NB) is quite complicated and is the subject of Appendix B. As seen by the notation, F is independent of time. Hence, F can be constructed during the setup process and stored. The apparent excessive attention to accuracy that is evident in determining the F array is necessary due to the large time steps that are used to limit numerical dispersion for DVM.

For the leg-to-leg ransfer option (see Section 2.4.9) particles are not allowed to skip a leg over a time step, thus only particles in the last leg can discharge over a time step. By replacing the path-averaged velocities with the velocities of the last leg, the process of finding discharge fractions for the leg-to-leg transfer option is identical to the leg-averaged option described in Appendix B.

2.4.8 Distribution of Source Into Grid Blocks

The source model determines the total amount of source for each isotope over time that is available for transport. In the flow-through source model, all material available for transport for each transport time step is injected evenly into the source leg grid blocks, where the source leg is the first leg in the migration path. Consequently, for transport, NEFTRAN II requires at least two legs in the migration path; the first leg contains the source blocks and all subsequent legs the transport path. Distribution of source particles into the grid blocks using a mixing-cell source is quite complicated and is described in detail in Appendix C. The basic premise is that particles leaving the mixing cell are given a velocity using DVM as they exit the mixing cell, and allowed to travel as far as they will go over the time remaining in the transport time step. As particles exit the mixing cell into the migration path, the scheme takes into account radioactive decay and differing species velocities. Similiar to DVM transport and discharge, sets of fractional multipliers are developed for grid blocks that receive source particles over a time step.

2.4.9 Leg-to-Leg Transfer Model

Section 2.4.2 discusses the implementation of the DVM transport model based on the assumption of a single one-dimensional homogeneous leg representing the entire migration path for radionuclides. In others words, even though each leg in the migration path may represent a different medium, the velocities in each leg are averaged and the DVM transport model is applied to the averaged velocity with a single dispersivity. For saturated porous media, combining different velocities into a single average velocity has been shown to yield acceptable results and to be computationally efficient (Campbell and others, 1981). However, if some of the legs are to represent fractured media with the accompanying diffusion into the rock matrix, the contact time between fluid in the fracture and matrix becomes important. The contact time induced by using a velocity averaged over both porous and fractured legs may not be physically meaningful. Also, to simulate transport in both unsaturated and saturated media, the dispersivity for each zone may be significantly different such that using DVM based on a single dispersivity may not be appropriate. Therefore, the DVM transport model has the capability to include the concept of transporting radionuclides between different legs over a time step (i.e., leg-to-leg transfer). Within each leg, the DVM concept of distributing velocities is implemented as discussed in Section 2.4.2.

The simulation of leg-to-leg transfer of radionuclides must account for particles that begin a time step in one leg and end the time step in another. For the leg-to-leg transfer model, the magnitude of the time step is restricted such that a leg cannot be skipped over the time step (see Section 2.4.3). Consequently, particles with a given velocity that begin the time step in a certain leg are assumed to either end the time step in that leg or in the next leg. As mentioned previously, with only one exception (discussed at the end of this section), particles that do not exit a leg in a time step are accounted for in the same way as described in Section 2.4.2.

Leg-to-leg transfer is complicated by the possible occurrence of negative velocities in the distribution of velocities for each leg. Negative velocities can occur due to the assumption that solute dispersion can be modeled assuming a Gaussian distribution of velocities. This is the conventional treatment of dispersion and is a property of the mathematical formulation, not the physical process. The physical process of mechanical dispersion (i.e., excluding molecular diffusion) can only result in movement of material downstream in the direction of flow and not upstream. For the leg-to-leg transfer model, if negative velocities are encountered, particles are not allowed to travel backwards into the previous leg in the migration path. This is accomplished by attaching "catcher" blocks at the leading edge of each leg. The use of catcher blocks in the leg-to-leg transfer model will be discussed at the end of this section.

The occurrence of negative velocities causes one further difficulty for implementing the DVM leg-to-leg transfer model. It requires that the code track the leading and trailing edges of a contributor block forward in time to see if there is any overlap with the given receiver block. This is different than the implementation of DVM for the path-averaged case, where the code tracks backwards in time from receiver blocks to find all possible contributor blocks.

The need for this altered approach is due to the possibility that contributor blocks may be undefined for some receiver blocks. In other words, every receiver block in a new leg may not have a source block from the previous leg. This happens when a packet of particles ends up straddling a leg boundary. If the velocity of the particles is less than zero in the first leg and greater than zero in the second leg, the original contents split into two separate packets. Consequently, the partial packet that travels backwards in the first leg does not contribute to the expected receiver block in the second leg and the source for these receiver blocks becomes undefined. Thus, it is easier in the leg-to-leg transfer model to track particles forward in time rather than to search backwards for contributor blocks.

Intuitively, the logical time to check when a packet may straddle a boundary should be at the end of a time step. However, due to radioactive decay, the time when a packet may straddle the leg boundary is checked after the time spent as such isotope. This time is discussed in Section 2.4.6. For example, for the subchain $I_1 \rightarrow I_2 \rightarrow I_3$, the time the packet is straddling the leg boundary after T_1 , the time spent as I_1 , is significant.

Before discussing the scheme for tracking packets forward in time in the leg-to-leg transfer model, the general set up of NEFTRAN II will be discussed. A packet is defined as the fraction of material in a contributor block that begins the time step as isotope i, I_i , and ends the time step as isotope p, I_p . For example, the decay chain $I_1 \rightarrow I_2 \rightarrow I_3$ will have six packets in each contributor block corresponding to the subchains:

- 1) I1 + I1
- 2) I1 + I2
- 3) 12 + 12
- 4) $I_1 \rightarrow I_2 \rightarrow I_3$

- 5) I₂ → I₃
- 6) 1₅ → 1₅

The fraction of material contained in a packet, b, is

$$f_b \approx M_k DP[1_1 \rightarrow \tilde{1}_p, t], \qquad (2.88)$$

where M_k is the material in contributor block k and DP[$I_i \to \widehat{i}_p,$ t] is the decay production factor.

For the leg-to-leg transfer model, to track a packet forward, the progress of the packet as species I_i for time T_i is first tracked. Then the packet is tracked as it migrates with the velocity of species I_{i+1} for time T_{i+1} and so forth. If packet b ends T_i with both leading and trailing edge in the same leg, the location for packet b is updated and stored. If the packet ends T_i straddling a leg boundary, the packet is split into two new packets and relevant information is stored. Each new packet is characterized by:

- a, the location of its leading edge,
- b. the location of its trailing edge, and
- c. the fraction (geometric mixing fraction) of the original packet that the new packet represents.

At the end of the time step, it is determined whether any of the packets, old or new, overlap receiver blocks. This information is important in order to find the appropriate geometric mixing fractions for the potential receiver blocks.

To find the geometric mixing fractions for contributions from blocks in leg L to receiver blocks in the next leg (L+1), the leg-to-leg transfer model accounts for the following four different overlap possibilities (illustrated in Figure 2.13):

- a. both the leading and trailing edges of packet b are located in receiver block i,
- b. the leading edge of packet b is in receiver block i, but the trailing edge is not.
- c. the trailing edge of packet b is in receiver block i and the leading edge is not, or
- d. the leading and trailing edges of packet b envelope receiver block i.

If none of the conditions (a) - (b) are true then there is no overlap and the geometric mixing fraction for receiver blocks in the next leg is zero.



Figure 2.13. Illustration of Four Possible Situations Arising Because of an Overlap of a Packet and a Given Receiver Block

As indicated previously, another topic that needs to be addressed for leg-to-leg transfer is when a negative velocity dictates movement from leg L to leg L-1. To account for these negative velocities, the leg-toleg transfer model artificially extends the length of leg L to "catch" the negatively directed particles. Figure 2.14 shows three such catcher blocks appended to leg L. Particles in leg L-1 have a velocity distribution calculated with Equation 2.59 using the pore velocity, dispersivity and retardation of leg L-1. As these particles arrive at the boundary between leg L-1 and leg L, they are subject to the velocity distribution in leg 1 corresponding to the pore velocity, dispersivity and retardation of leg L. The velocity distribution in leg L may have negative components that will force particles backwards into leg .1. However, this is not allowed because once particles leave leg L-1 they are no longer transported with the properties of that leg. Instead, catcher blocks are added to the entry of leg L to allow particles to move backwards and be transported with the velocity distribution of leg 1. without actually going back into leg L-1. After each time step, the particles that are in the catcher blocks are summed and put into the first grid block of leg L. This ensures that no particles are allowed to migrate farther back in the artificial catcher blocks.

There is a potential inconsistency in the treatment of particles near a leg boundary. This inconsistency can occur for a velocity packet in which the parent velocity is positive and the daughter velocity is negative. An example is a two member chain for which this occurs for at least one packet. In this case the packet splits and part of the original packet remains in leg L and part remains in leg L+1. However, for transport in the interior of leg L, the fraction contributing to the last grid block is larger than what it is supposed to be. In fact, the entire distance from the trailing edge of the packet to the leg boundary is available for interior transport since the packet maintains the velocities for leg L throughout the time step. Thus, not allowing particles to return to their original leg can result in double counting by the interior transport fraction near the boundary.

To correct for the above special case, an algorithm was developed to adjust the amounts of particles that remain in each leg. For each subchain that has more than one member, the need for adjustment is checked. If a velocity interval is detected having some positive movement followed by some regative movement, the contributions from block to block in the leg interior near the down-gradient boundary are traced. If necessary, an adjustment fraction is generated and saved. This algorithm is also applied to the last leg to avoid inconsistent treatment with the discharge model discussed in Section 2.4.7.

2.4.10 Matrix Diffusion Model

NEFTRAN II contains a model that treats the exchange of radionuclides between a mobile dynamic fluid and an immobile stagnant fluid in conjunction with the DVM transport model. An example of where this model may be applicable is in simulating radionuclide transport from fractures to the surrounding rock matrix. The expected effect of this phenomenon on the





transport of stable species is to cause dispersion of the species. For decaying species the retention period in the immobile phase may be long enough to reduce concentration through radioactive decay significantly. This model may also be applicable for simulating transport in porous media that contains dead-end pores.

Theory. The matrix diffusion model contained in NEFTRAN II is based primarily on the work of van Genucheen and Wierenga (1976). The model uses the simplifying assumptions of a constant immobile pore volume to represent the immobile phase and a mass exchange coefficient to determine the mass flux between the mobile phase and the immobile phase.

The rate of diffusion from the mobile phase to the immobile phase is assumed to be directly proportional to the concentration difference between the mobile and immobile phases. Letting subscript d (dynamic) denote mobile phase properties and subscript s (stagnant) denote immobile phase properties, the governing mathematical equation for the rate of change of concentration in the immobile phase is

$$\theta_{s} R_{s} \frac{\partial C_{s}(\mathbf{x}, t)}{\partial t} = \beta \left[C_{d}(\mathbf{x}, t) - C_{s}(\mathbf{x}, t) \right]$$
(2.89)

where C denotes concentration in units of mass per unit volume and the constant of proportionality, β , is the mass exchange coefficient with units of inverse time, θ is the volume fraction occupied and R the retardation factor.

Implementation. As discussed above, van Genuchten and Wierenga (1976) account for the loss of solute from the mobile fluid to the immobile fluid by the addition of a sink term to the convective-dispersion equation. Since time is discretized in DVM, this fracture-matrix exchange can be included at the end of each time step. That is, particles are transported in the mobile phase using the conventional DVM solution of the convective-dispersion equation. At the end of a transport step, concentrations in the mobile phase are compared to those in the immobile phase and diffusional exchange is modeled.

For those legs along the migration path that the user selects as representing dual-porosity media, a parallel system of grid blocks is generated. The only mechanism for molecules to move from one system to the other is by diffusion. Figure 2.15 shows leg L with its associated immobile phase. As indicated in Figure 2.15, the Kth block of leg L is associated with the Kth block containing immobile fluid for leg L. Thus, exchange occurs between pairs of blocks in the two systems. No exchange occurs between adjacent immobile phase blocks.

For each block pair, the rate of diffusion is assumed to be directly proportional to the concentration difference between the mobile and immobile phases, as indicated in Equation 2.89. A forward finitedifference approximation of the time derivative in Equation 2.89 yields



Figure 2.15. Illustration of Adjacent System of Grid Blocks Simulating the Rock Matrix in Dual-Porosity Legs

$$C_{g}(x,t+\Delta t) = \frac{\beta}{\theta_{g}} \frac{\Delta t}{R_{g}} \left[C_{d}(x,t) - C_{g}(x,t) \right] + C_{g}(x,t)$$
(2.90)

Incorporation of Equation 2.90 into DVM requires that particles in a given grid block are converted into concentrations. Allowing for retardation, this conversion is as follows

$$C_{d}(x,t) = \frac{P_{d}(x,t)}{\theta_{d} R_{d}}$$

$$C_{g}(x,t) = \frac{P_{g}(x,t)}{\theta_{g} R_{g}}$$
(2.91)

where P(x,t) is the quantity (in atoms) of the given species at location x and time t, R is the retardation factor and θ is the volume fraction occupied.

Using Equation 2.90 and Equation 2.91, the number of atoms in the stagnant region at t + Δt is

$$P_{g}(x,t+\Delta t) = \left\{ \frac{\beta}{\theta_{g}} \frac{\Delta t}{R_{g}} \left[C_{d}(x,t) - C_{g}(x,t) \right] + C_{g}(x,t) \right\} \theta_{g} R_{g} . \quad (2.92)$$

To complete the solution, the concentration in the dynamic fluid must also be updated. This is done by conserving mass (atoms) between the immobile and mobile phase before and after diffusional exchange. That is

$$P_{d} = P_{T} - P_{s} \qquad (2.93)$$

where $P_{\rm T}$ is the total number of atoms in the system (mobile plus immobile) before diffusional exchange.

After P_d is found, the value of $P_n(x, t \notin \Delta t)$ is updated to account for radioactive decay. The spatial distribution of particles in the mobile phase at time t + Δt is calculated using the approaches discussed in Section 2.4.2.

To summarize, the implementation of the fracture-matrix exchange algorithm is as follows:

- transport radionuclides in the mobile phase from t to t + At,
- (11) calculate exchange for each nuclide using Equations 2.90 through 2.93,
(111) in preparation for the next time step, age the stoms in the immobile fluid to t + 2Δt,

(iv) set t = t + Δt and return to (1).

Those steps are repeated until an upper bound time is reached. Step (iii) insures that radionuclides aged to the same time in both phases are interchanged.

The implementation of step (ii) uses Equations 2.90 through 2.93 with location x governed by grid block number. There is one added complication, however. Since the time steps for DVM are typically large, straightforward use of Equation 2.90 can result in concentrations modified beyond the point of equilibrium. Thus, NVFTRAN II requires the concentration difference between the fractures and the matrix not to change sign over At. So if, for example,

$$d_d > C_g$$
 (2.94)

and after accounting for diffusional exchange, it is found that

then exchange should have ceased when equilibrium was reached. The equality

$$C_d = C_s$$
 (2.96)

is imposed whenever this occurs.

2.4.11 DVM Transport in Time-Dependent Velocity Fields

The most significant difference between NEFTRAN II and NEFTRAN is the NEFTRAN II capability to transport radionuclides in time-dependent velocity fields. Specifically, NEFTRAN II simulates time-dependent velocity fields by approximating the time-varying velocities with sequential steady-state velocities. The user defines time ranges over which the velocity in each leg is essentially constant and these velocities are read into NEFTRAN II from an external file (see Section 4.3.1). As diacussed in Section 2.4.2, the only difference in implementation of DVM for time-dependent velocities is following each time interval, the code recomputes the transport fractions based on the new velocities and new time steps to be used for the next time interval.

This capability was added to NEFTRAN as a first approximation to modeling transport in unsaturated media. For unsaturated-zone cransport, transport parameters become time dependent. For example, saturation is a

function of time and, therefore, the retardation factor and velocity, as they are a function of saturation, are also time dependent. Although radionuclide transport in the unsaturated zone is complex and may not be completely defined at this time, this first approximation may be used to mimic the effects of transport in the unsaturated zone, and still retain the efficiency of the code needed for up formance assessment requirements. It is also possible that, for corticle combinations of parameters, this approximation is acceptable.

Besides modeling unsaturated-zone transport, this consulity can also be used to model significant climatic changes that result in ground-water velocity changes. For example, one could assume that, over a period of 10000 year, the climate changes at 5000 years such that the flow velocities are doubled. However, the basic underlying assumption is that the flow paths do st change with time (i.e., the migration path is constant with time), and only the magnitude of the velocity is time dependent.

<u>Time-dependent</u> <u>turation</u>. As indicated above, for transport in the unsaturated zone, we retardation factor is a function of saturation (n_g) which is time-dependent. To be able to mimic this effect. NEFTRAN If allows the user to is put time-dependent saturations along with timeint velocities. The only effect that saturation has is on the infactor. (R), where the unsaturated retardation is ctor is given by

$$R_{unsat} = n_s R$$
, (2.97)

This is a fine approximation to the effects of the unsaturated-zone transport on reduction; however, it would be simple to incorporate another relationship not necessarily based on saturation, as long . We effect on revertation is linear.

Besides being used to model unsaturated-zone transport, this capability could be used to mix c a linear time-dependent geochemical effect on retardation. For example, if the retardation factor was assumed to be a linear function of mineral composition and, the composition was depleted with time, this capability could be utilized.

3.0 DESCRIPTION OF CODE

The following sections will describe how N°FTRAN II is structured, as well as the subroutines, the parameter state. nis and the common blocks contained in the code.

3.1 Structure

The code structure will first be described in general, including the structure that is followed for multiple simulations. Next, the structure of the source module and the transport module contained in NEFTRAN II will be discussed.

3.1.1 General

A flow chart of the general structure of NEFTRAN II is shown in Figure 3.1. The first task that is executed by the main program is to call a subroutine to read the input file(s) provided by the user. Next, if the user has requested for NEFTRAN II to solve the fluid flow network, the network flow mode? is implemented by calling the appropriate subroutines. The next function of the main program is to implement the source model contained in NE.TRAN II. The source model provides the source rates that are required by the DVM transport model, but is independent of the DVM transport model. The final step in the simulation is radionuclide transport. For multiple chain simulations, the DVM transport model is implemented inde, endently for each chain. After all chains have been transported, the last task of the main program is to call a subroutine to write the discharge rates for rach isotope to the appropriate output files.

Automated multiple simulations in NEFTRAN II can be accomplished b, two different means. First, a completely new input file or parts of the input file can be read for each new simulation based on certain input options (see Section 4.5.1). Consequently, if the user wanted to run multiple simulations for completely or partially different input sets, one could simply append all of the input sets into one input file, with the appropriate options indicated between each data set. NEFTRAN II would execute each data set until an end-of-file was encountered.

Second, specific input can be over-written based on data from an external file (see Section 4.3.1 for a description of this file). This is termed the statistical Monte Carlo run mode of NEFTRAN II, where the external file contains vectors of randomly sampled input variables found from a computer code like LHS (Iman and Shortencarier, 1984). Each vector contains one value for each of the set of sampled data input variables. For the statistical run mode, NEFTRAN II reads input data from the basic input file, and if the user has requested for sampled data to be read from an external file, it replaces the input data parameters with values from the external file. This is repeated for each sampled vector until an end-of-file is encountered in the external file. The reader should note that these two ways of conducting multiple simulations with NEFTRAN II are not mutually exclusive and although not normally done, both could be implemented at the same time if this was required by the user.



3.1.2 Source Module

Figure 3.2 shows a flowchart of the source module contained in NEFTRAN II. The module loops through time based on source time steps. The first process that is accounted for over a time step is leaching. If leaching is the only process being considered (as specified by the user) then the source rate can be determined based on the amount leached for either the flow-through source or the mixing-cell source, whichever model is being implemented. However, if the solubility-limit of the source is also being modeled, then the amount leached is added to the undissolved inventory. Next, if there is a time-dependent flow rate through the source, the total flow rate over the time increment is found. This is needed in the next step where the amount dissolved, based on solubility limits is found. Next, a comparison between the amount dissolved based on solubility limits and the amount left in the inventory is made.

The amount placed in the dissolved inventory is the minimum of these two quantities. This amount dissolved is then subtracted from the undissolved inventory. At this point the source rates can be found for either the flow-through source or the mixing-cell source, again, depending on which model is being utilized. After the source rates are found, the inventory is updated for the next time step, and the time is incremented. If the incremented time is greater then the problem simulation time, the source module terminates its calculations.

3.1.3 Transport Module

Figure 3.3 presents a flowchart of the transport module contained in NEFTRAN II. If the analytical solution is being implemented for simulating transport, the appropriate equations (Equation 2.18 - Equation 2.22) are solved. If the DVM transport model is being utilized to solve for transport, for time-dependent velocities, transport is simulated for the first time interval. If the fluid velocities are not time-dependent, only one time interval occurs and this interval is from the release time to the problem simulation time. Before the simulation actually occurs, the transport fractions can be found. If the mixing-cell source model is being implemented, the fractions relating the distribution of the source in the transport path can be found as well as the leg-to-leg transfer fractions, if the leg-to-leg transfer algorithm is being implemented. Finally, before actually simulating transport, the discharge fractions are found. During the simulation, for each time step, matrix diffusion is accounted for if the user has indicated that some of the logs in the transport path are dual-porosity legs. The transport simulation is terminated when the time is greater than the time interval. If the time interval is greater than or equal to the problem simulation time, the transport module calculations are stopped. Otherwise, the transport fractions are found for the next time interval and transport is simulated for that time period.

3.2 Subroutines

The following sections will briefly describe the function of each subroutine contained in NEFTRAN II, as well as where the subroutine is called from and what subroutine(s) it calls. The first subroutine that



á

4

-

6

0

Figure 3.2. Flowchart of Source Module in NEFTRAN II



.

Figure 3.3. Flowchart of Transport Module in NEFTRAN II

1

1990 (F) 1990 (F)

9

is discussed is the main driving program (NEFMAIN) and subsequent subroutines are discussed in alphabetical order.

3.2. NEFMAIN - main program

Callad		4	The second		dia.	in.			
1.155	a.,	£.	€2	QL	12	τ.	Ø	50.	

Calls BSOLVE, CHAIN, COEFF, FLOWIN, GETRV, METHOD, PTHLEN, SOURCE, WORK

NEFMAIN is the main driving program of NEFTRAN II. It is capable of handling single or multiple simulations. It calls FLOWIN in which the data input is read. For multiple runs, the initial call to FLOWIN serves as the basic set up. Subsequent runs can be accomplished by either calling FLOWIN for additional data sets or GETRV to read input vectors from an external file (unit 10) and overwrite existing data (for a discussion of this external file see Section 4,3,1). If the user opts for the flow network to be solved, NEFMAIN calls COEFF and BSOLVE, checks an error flag to see if BSOLVE was successful in solving the pressure equations, and condenses the pressure array since some of the pressures are known from input. NEFMAIN calls PTHLEN to calculate pore fluid velocities if the flow network has been solved, or to check the user input velocities for flow direction consistency. These velocities are required by the transport model. Next, NEFMAIN implements the source model by calling SOURCE. The source model is decoupled from the transport model and provides source rates for the DVM transport model. If the analytical transport option is chosen, SOURCE updates the user-specified inventories to release time and exits. For each chain, NEFMAIN calls CHAIN and METHOD to implement the transport model. After the transport simulations are completed for each chain, NEFMAIN calls WORK to write discharge information to the appropriate output file (unit 30).

3.2.2 ADJB(VA, LG, IP, TS, ILAST, KNT)

Called From FACER

Calls

Subroutine ADJB is implemented with the DVM transport model in conjunction with the leg-to-leg transfer option. When the leg-to-leg transfer algorithm is invoked in FACER, negative velocities (see Section 2.4.9) can cause double counting of some particles at the end of each leg. Subroutine ADJB is called from FACER to compute the fractions to correct for this double counting for each leg.

3.2.3 BAND(TSTART, TEND)

Called From METHOD

Calls GIT, RATIO, TPPRT

Subroutine BAND is called from METHOD when the user opts for the analytical transport model (see Equation 2.1? - Equation 2.22). BAND applies the analytic solution for a chain of up to three radionuclides with equal retardation factors at a prescribed distance from the source. The source boundary condition is a point source in space and a decaying band in time.

3.2.4 BRANCH(EPS)

Called From		Calls
SOURCE, DTUPDT,	SETUP	ET

Subroutine BRANCH creates the radioactive decay subrains that are used to estimate decay/production of an isotope over a time step and calls ET to find the decay/production factors (as far upchain as necessary) based on the Bateman equations. SOURCE calls BRANCH to update the radionuclide inventory to the release time, DTUPDT calls BRANCH to age the inventory over the initial source time step, and SETUP calls BRANCH to age the inventory by the DVM transport time step.

In creating the subchains, BRANCH traces branches from an isotope upchain to the end of the chain(s). The current code logic allows four such paths. BRANCH determines how far upchain to look for reasonable representation of the production of the isotope over a time step using ratios of Bateman production/decay factors. EPS is the maximum cutoff ratio. When called from SOURCE, EPS is 10^{-8} , when called from DTUPDT, EPS is 10^{-5} , and when called from SETUP, EPS is 10^{-4} . Terminating a subchain prior to a branch point decreases the number of necessary paths. For a detailed discussion of how NEFTRAN II stores decay chain information, which is implemented in subroutine BRANCH, see Appendix D.

3.2.5 BSOLVE(KER)

Called	From	Calls
NEF		$a_{i}=a_{i}+a_{i}$

Subroutine BSOLVE is called from NEF when the network flow model is implemented. BSOLVE solves the banded matrix equation set up in subroutine COEFF using a Gaussian elimination technique. This subroutine precludes the need to use an external subroutine package to solve the matrix equation.

3.2.6 CATCH(GA, NPT, VDT)

Called From Calls DXDT

For the DVM transport model, subroutine CATCH determines the maximum distance (VDT) that will be required to catch negative directed particles for each leg. DXDT and CHAIN use this distance and the space step to determine the total number of catcher blocks needed for each leg.

3.2.7 CHAIN(IW)

Calle	d From		Calls	
NEF,	SOURCE		DXDT,	TRACER

Subroutine CHAIN substitutes information for a given chain in a multiplechain execution to local arrays. When called from SOURCE (IW \neq 0), CHAIN calls TRACER to find the mean travel times for each isotope which are used by DTUPDT to determine isotope importance for source time step determination. When called from NEF (IW = 0), CHAIN calls TRACER to determine mean travel times to be used by DXDT for transport time step determination. For the DVM transport model, CHAIN also calculates the number of catcher blocks needed for each leg. For time-dependent velocities, CHAIN saves the minimum space step required and the maximum distance required to catch negatively directed particles for each leg for all time frames, and checks to make sure dimensions are not exceeded based on these parameters.

3.2.8 CHKPTH

Called From		Calls
PTHLEN		*****

Subroutine CHKPTH is called by PTHLEN to verify that flow is downgradient along the user-input migration path. It also checks that legs along the migration paths are sequentially connected.

3.2.9 COEFF

Ģ	alled From			Calls
N	EF			

COEFF is called when the network flow model is implemented and puts into matrix form the system of equations used to solve the flow network (see Section 2.1). Specifically, COEFF creates the transmissivity matrix and the constant vector used in solving for the unknown pressures at leg junctions. COEFF also implements the viscosity submodel.

3.2.10 DTUFDT

Called	From			Calls	
SOURCE				BRANCH,	ET

DTUPDT provides the time step for the source model calculations if it is not input by the user. Section 2.3.2 presented the basic criteria for time-step determination and discussed the specific parameters that DTUPDT applies in finding the time step for source calculations. By calling BRANCH and ET, DTUPDT also finds subchains and decay/production factors over the source time step.

3.2.11 DXDT

Called	From		Calls
CHAIN			CATCH

DXDT finds the space and/or time step for the DVM transport model if they are not input by the user. Material is presented in sections 2.4.3 and 2.4.4 that discusses the basic criteria for space- and time-step determination and discusses the structure of DXDT and how it applies the set of criteria to determine the time and space increment. DXDT calls CATCH to find the maximum distance that will be required to catch negative directed particles for each leg.

3.2.12 ET

Called	From		Calls
SETDIS,	BRANCH,	DTUPDT	RATIO

Function ET is used to evaluate the Bateman coefficients for calculating the radioactive decay/production factors. When called from BRANCH, ET finds the factors for either updating the source inventory to release time or for updating the inventory by the DVM transport time step or the source time step. When called from SETDIS, FT finds the decay/production factors for isotopes surviving decay to discharge. When called from DTUPDT, ET finds the decay/production factors over one half the source time step. ET uses a Taylor's series expansion to solve for the Bateman coefficients. If convergence of the Taylor's series is expected to require too much execution time (i.e., a combination of small half-lives and large time-step), ET calls RATIO to evaluate the Bateman coefficients in a pairwise manner.

3.2.13 FACER

Called	From		Calls
SETUP			ADJB

Subroutine FACER implements the leg-to-leg transfer algorithm for the DVM transport model. FACER finds the leg interface fractions for each isotope in each subchain crossing from a leg to the subsequent one. For velocity packets that are negatively directed, FACER calls ADJB to adjust the fractions to ensure that double counting does not occur at the leg interfaces.

3.2.14 FLOWIN(IPASS, ROOT, KROOT)

Called From	Calls	
NEF	INPRIN,	STOPPER

Subroutine FLOWIN reads in all of the data input required by NEFTRAN II, with the exception of GETRV (see next section). For multiple data sets, IPASS > 1, FLOWIN re-reads only the input indicated by the INP array (see Section 4.5.1), and if an end-of-file is encountered it is assumed to signify a normal termination. On the first pass (IPASS = 1), FLOWIN opens the input and output files, centers the title and finds the execution date and time. For chains that are not included in the source calculations, (see Section 4.3.2), FLOWIN condenses the appropriate arrays. FLOWIN also calls STOPPER to do general data input checking.

For the PC version of NEFTRAN II, ROOT is a character string input by the user for the name of the input file ((root).INP, unit 2) not including the extension of the file name. ROOT is then used by FLOWIN to access other input files if required and to name output files accordingly.

KROOT is a counter that is used to count how many characters are contained in the character string ROOT. See section 4.1 for a more detailed discussion of the file naming scheme for NEFTRAN II.

3.2.15 GETRV(JTRIAL)

Called	From	Calls
NEF		STOPPER

GETRV is used in performing multiple simulations for statistical studies which allows the user to assign selected sampled values to the appropriate NEFTRAN II variable names. Consequently, for the most part, GERTV is a user-written subroutine and the user is responsible for the required replacement statements and units conversion factors. GETRV reads the external file (unit 10), which contains each statistical trial vector. Simulations are conducted automatically for each vector, where the selected input is over-written with the vector values for each simulation based on the user-supplied replacement statements. JTRIAL is read from the external file for each vector, and indicates the trial or vector number. An end-of-file encountered in the external file indicates normal termination for a statistical run. The format for the external file is discussed in Section 4.3.1.

3.2.16 GIT(T, Y, V, AL)

Called	From		Calls
BAND			

Function GIT is called from BAND and uses a fifth-order Hastings approximation (Abremowitz and Stegun, 1965) to calculate the sum of the complementary error function terms given in Equation 2.22. The complete analytical transport model solution is generated in BAND.

3.2.17 INPRIN(MM, INCRM)

Called	From	Calls
FLOWIN		

INPRIN prints user opted input parameters to the hardcopy output file. Some of the parameters may have been altered in subroutine STOPPER due to input error checks, otherwise they are as input. MM indicates which parameter sets the user has designated to be printed and INCRM is a flag which indicates whether or not the default values are utilized for the space- and time-step determination parameters. INCRM equal to zero indicates that the default values have been used.

3.2.18 INTG(S1, B1, S2, B2, T1, T2, D, F, N, DT, ANS)

Called	From		Calls
MXCLL			****

Subroutine INTG is called from MXCLL and is accessed only when the mixing-cell source is used. INTG is used to evaluate the integrals in the mixing-cell source model developed in Appendix C. The variables in

the argument list are the limits of integration that are found in MXCLL and defined in Appendix C.

3,2,19 LECHMOD(T1,T2,F)

Called	From		Calls
SOURCE			\times + + + +

LECHMOD is part of the source model and is called from SOURCE. LECHMOD finds the total fractions unleached at times TI = t and $T2 = t + \Delta t$. The fraction, F, leached is the difference of these two fractions. Depending on user input, the fraction leached is either based on a constant leach rate or an exponentially decaying leach rate.

3.2.20 METHOD

Called From	Calls			
NEF	BAND,	SETUP,	TPPRT,	TRNSPT

Subroutine METHOD is the driving subroutine for the transport module. If the user selects the analytical transport model, METHOD sets the start time, stop time and time-step and calls BAND to solve the analytical transport model equations (Equation 2.18 - Equation 2.22). See Section 2.2.2 for a discussion on how the starting time, stopping time and timestep are found. Before calling BAND, METHOD checks to see if discharge occurs during the problem simulation time based on the average migration time for each isotope. If no discharge is detected then METHOD calls TPPRT to print out zero discharge information to the approviate output files at the release time (TRLSE) and the problem simulation time (TUB). For the analytical solution, METHOD also checks to see if the last rate is written at a time less than the problem simulation time. If this is true, METHOD calls TPFRT to print/append zeroes to the appropriate output files.

If the user opts for the DVM transport model, METHOD calls DXDT and SETUP to generate the parameters needed by TRNSPT. METHOD calls TRNSPT to simulate radionuclide transport through the migration path for the problem simulation time. For time-dependent fluid velocities, METHOD executes the above sequence of commands for each time frame.

3.2.21 MXCLL(KBMAX)

Called	From		Calls
SETUP			INTG

Subroutine MXCLL is called from SETUP when the source rate is distributed into the transport path based on a mixing-cell source region. MXCLL creates the source factor array used to update the fraction of the source of a given isotope to a specific grid block over a transport time step. MXCLL is structured according to the subcase numbering structure found in Appendix C. KBMAX is found in MXCLL and is the number of source grid blocks needed for the mixing-cell source. KBMAX is used in CHAIN to find the total number of grid blocks required for the source leg. 3.2.22 PRP(D, R, V, VP, DL, N, T1, T2)

Called From Calls

Function PRP solves the integrals that are needed by SETDIS to create the discharge factor array. The discharge factor array is needed by the transport module to determine the discharge rates at the end of the migration path. The variables contained in the argument list are found in SETDIS and are used in the limits of integration.

3.2.23 PTHLEN

Called	From	Calls	
NEF		CHKPTH,	TRACER

Subroutine PTHLEN is called from NEF and performs several tasks. First, if the flow network is solved, PHTLEN calculates the volumetric flow rates in each leg based on the pressures solved for in BSOLVE. At the user's option, PTHLEN prints pressures and flowrates of each leg in the network. Next, for the transport calculations, PTHLEN determines the pore fluid velocities for each leg in the migration path. PTHLEN calls ChKPTH to ensure that the pore velocities are consistent with the migration path (i.e., checks flow direction). For the averaged-leg DVM transport calculations, PTHLEN calculates the total path length from the source boundary to the discharge point. If the user opts, PTHLEN prints out path/velocity information after calling TRACER to find the nominal travel time, for steady-state velocities, or the mamimum distance the fluid travels for time-dependent velocity fields.

3.2.24 RATIO(DJ,DI,TIME,RAT)

Call	ed From	Calls
ET,	SETDIS	*****

RATIO is called from ET when the Taylor series approximation for finding the Bateman decay/production factors will require too much execution time to converge and is called from SETDIS to treat two-member production subchains. Ratio evaluates terms of the form

$$RATIO = \frac{e^{-\lambda_1 t} - e^{-\lambda_j t}}{\lambda_1 + \lambda_1} , \qquad (3.1)$$

where λ_i is the half-life of isotope i (DI), λ_j the half-life of isotope j (DJ), and t the time the decay/production factor is being found.

RATIO checks for extremes in half-life time products and for the smallness of differences in half-life values.

3.2.25 SETDIS

Called From SETUP Calls ET, PRP, RATIO Subroutine SETDIS is called from SETUP to create the discharge factor array. SETDIS finds this array by treating atoms that survive decay to discharge and by treating production subchains at discharge. To find atoms that survive decay to discharge, SETDIS calls ET to find the appropriate decay/production factors. To treat production subchains, an analytical treatment is used for two-member subchains. For this analytical treatment, SETDIS calls RATIO to find production/decay factors. For subchains having more than two members, SETDIS uses a velocity approximation scheme to treat subchains. To implement this approximation, integrals have to be evaluated and SETDIS calls PRP to evaluate the appropriate integrals. At the user's option, SETDIS prints out the discharge factor array to the appropriate output file (unit 6).

3.2.26 SETUP

Called Trom METHOD Calls BRANCH, FACER, MXCLL, SETDIS TIMER

SETUP is called from METHOD to establish the source, transport, and discharge fractions for the DVM transport model. Specifically, SETUP performs the following functions:

- Calls BRANCH to establish subchains for transport and find decay/production factors for the transport time step.
- 2. Distributes isotopic velocities normally with intervals of equal probability for each species in each leg.
- 3. Finds subchain velocities for transport by calling TIMER to find the mean time spent as each isotope for each subchain. This is only done when the number of isotopes input is greater than one.
- Prints the velocity and decay/production information to the output file (unit 6) if the user has requested this in the input.
- 5. Determines the transport fractions by finding the pointer array (JV) which points to contributor blocks, the multiplier array (B) which is used to transport the material and the number array (N) which contains the maximum entries of the pointer array. If the user opts in the input, the multiplier array and the pointer array will be printed to the output file (unit 6).
- 6. Finds arithmetically averaged subchain velocities to be used in the mixing-cell source model and discharge model.
- 7. If the mixing-cell source model has been used, SETUP calls MXCLL to find the source factor array. MXCLL returns KBMAX, which is the number of source blocks needed if the mixing-cell source modelis used.
- If the mixing-cell source model has been used, METHOD finds the total number of grid blocks needed based on KBMAX, and checks this total against the dimensions. If dimensions are exceeded but a

statistical run is not being conducted, the program is stopped. If a statistical run is being conducted, KBMAX is reduced according to the dimensions and a warning is printed to the output file.

- 9. If the leg-to-leg transfer algorithm is to be used, SETUP calls FACER to find the transport fractions at the leg interfaces.
- 10. If the user has requested on input, the DVM time and space increments, the total number of grid blocks and the total number of catcher blocks, and the source type are printed to the hardcopy output file (unit 6).
- 11. Calls SETDIS to find the discharge fractions for the discharge model used in the DVM transport calculations.

3.2.27 SIFT(NSORT, TSCL)

Called From WORK

Calls

If the user requests, discharge rates for all isotopes in each chain are placed on the same time scale in WORK. WORK calls subroutine SIFT to sort the times into ascending order.

3.2.28 SOURCE(IPASS, JTRIAL)

Ca	11	ed	Fr	om		
NE	F					

Calls BRANCH, CHAIN, DTUPDT, LECHMOD

Subroutine SOURCE implements the source model contained in NEFTRAN II by performing the following functions:

- 1. Calls BRANCH to update the waste inventory to the release time and prints release time inventory if the user has requested this on input. If the analytical transport model is being utilized, this is the only function performed by SOURCE.
- 2. Initializes the binary file (TAPE24, unit 24) of source rates that will be used by the DVM transport model.
- If the time-dependent velocity capability of NEFTRAN II is being 3. utilized, SOURCE intitalizes the relevant variables for interpolating the time-varying flowrate through the source regime.
- 4. Calls DTUPDT to find the sourc "ime step (if the user has not input one) and to age the inventory by the initial source time step.
- 5. If leaching is not included in the source model, depending on user input, SOURCE puts all the initial inventory into the leached-butundissolved inventory. If leaching is included in the source model, SOURCE calls LECHMOD to account for leaching between the leach time (inverse of the input leach rate) and the release time.

- 6. Sets up the mixing-cell ratios to be used to determine source rates, if the source is being modeled as a mixing cell, and updates these ratios to the midpoint of the source time step for reporting.
- If the source is a mixing cell and some leaching has occurred up to release time, SOURCE initializes the mining-cell concentrations based on the leached-but-undissolved inventory.
- 8. If the source is solubility-limited, 'nen SOURCE updates the mixing-cell concentrations based on solubility-limits applied to the undissolved inventory. SOURCE subtracts the dissolved amount from the undissolved inventory.
- Loops over source time steps. Subsequent steps are executed for each time increment.
- 10. Calls LECHMOD, if leach-limited source, to determine the amount leached over the time increment. This amount is added to the undissolved inventory.
- 11. If the source is a flow-through source and is only leach-limited, then SOURCE determines the source rate based on the amount leached during the time increment and the undissolved inventory. If the source is a mixing-cell source at is only leach-limited then SOURCE determines the source rate based on the amount leached, the mixing-cell ratios, and the flow rate through the source.
- 12. Finds total flow over the time increment by interpolating, if time-dependent flow rate through the source regime are being used.
- 13. Finds total amount dissolved based on solubility limits and the flow rate through the source and compares this amount to the current amount available in the undissolved inventory. The inventory dissolved is the minimum of these two amounts. Subtracts the dissolved amount from the undissolved inventory for the next time step.
- 14. Writes the source rates to the binary file (TAP24, unit 24) to be used by the DVM transport model and also to the appropriate output file (unit 25) if the user has opted for this on input.

15. Ages inventory by the source time step for the next time step.

3.2.29 SRCIN(T, SR1, SR2, TS1, TS2, N1, N2, NTOTX, S24, IEOF)

Called From TRNSPT

Calls

SRCIN is called from TRNSPT to get the source rate over the transport time step and place it into the appropriate blocks in the first leg of the migration path (the source leg). SRCIN finds the total source per isotope for each transport time increment by interpolating the rates from the binary source rate file - itten by SOURCE (TAPE24, unit 24). This is necessary since the source and transport models are run independently and will not necessarily have the same time step. The variables listed in the argument list are used for the interpolation.

For the flow-through source model, SRCIN sums the atoms that are currently in the source blocks, adds the source rate found for the time step increment, and uniformly distributes the total amount into the source blocks. Also for each time increment, SRCIN sums the atoms that are in the source-leg catcher blocks, adds this sum to the total sum that is to be distributed uniformly, and sets atoms in the catcher blocks to zero. For the mixing-cell source, the source is distributed into grid blocks in the migration path according to the source factor array found in MXCLL.

3.2.30 STOPPER(ISTOP)

Called 1	From			Calls
FLOWIN,	GETRV			****

STOPPER is called by FLOWIN and GETRV to check input data for consistency. STOPPER detects both fatal and non-fatal input errors and writes either stop messages or warning messages. NEFTRAN II, unlike its predecessors, does not use numbered stop statements, but a descriptive reason for program termination is provided on both the terminal screen and the hardcopy output file. ISTOP is a flag that indicates which parameter set is being checked. The only data set that currently is not checked by STOPPER is the increment-determination parameters.

3.2.31 TIMER(KNT)

Called]	From	Calls
SETUP		TSPFAC

TIMER is called by SETUP to find the mean time spent during a time step as each isotope for each subchain (see Section 2.4.6). SETUP uses this information to find the subchain velocities needed for the DVM transport model. For a chain of five members or less, SRCIN does the calculation directly by calling TSPFAC. For chains of more than five members, TIMER estimates the time using an approximation scheme. If requested by the user in the input, TIMER prints the fractions of DT spent as each isotope.

3.2.32 TPPRT(TM, TSET)

Called From BAND, METHOD, TRNSPT Calls

TPPRT prints the discharge curves determined from the transport simulations to the hardcopy output file at a time frequency of IFREQ (input parameter), depending on a user input option. If the user also opts for the discharges rates only to be written to a file (unit 30), then TPPRT writes the discharge curves to temporary local files (unit 15 - 20, one file for each chain in the simulation), where the unit number is a function of the chain index. These local files are then used by WORK to write the final discharge rate file.

TPPRT is called from BAND every time step increment to print discharge curve points found using the analytical transport model. When called from TRNSPT every time increment, TPPRT prints discharge curve points found using the DVM transport model. In METHOD, if no discharge is detected during a simulation time for the analytical solution, TPPRT is called to print zero discharge points at the release time and the simulation time. _PRT is also called from METHOD for the analytical transport solution, to append zeroes to the output files (unit 6 and/or unit 30), when TEND is less than the simulation time.

TPPRT converts the output from the transport models from atoms/yr to Ci/yr, where less than one atom/yr is considered exact zero. TPPRT also finds the time of the initial breakthrough, the total discharge and the peak discharge rate and time of occurrence for each isotope. In the argument list, TM is the time at which the discharge rate for each isotope is printed. TSET is a variable that is used to make the times at discharge is written consistent with the time source is assumed to be available for transport.

3.2.33 TRACER(K, TT, PDIS)

Called From CHAIN, PTHLEN Calls

TRACER is called from PTHLEN (K=0) to find the mean fluid travel time (TT) for steady-state velocity fields, and for time-dependent velocity fields, TRACER finds the maximum fluid travel distance (PDIS). When called from CHAIN, TRACER finds the mean isotopic travel time (K = isotope index).

3.2.34 TRNSPT(T, TSET, NTP, NPT, KALL)

Called From METHOD

Calls SRCIN, TPPRT, XCHNG

TRNSPT is the DVM transport routine that performs the necessary multiplications to transport material over grid blocks for each time increment. TRNSPT accomplishes interior leg transport, leg-to-leg transport, and discharge by using multipliers developed in SETUP. TRNSPT loops over time from the time of source release to the upper time bound specified by the user. If time-dependent velocities are used, TRNSPT loops over time within each time interval. Within the time loop, TRNSPT performs the following functions:

- 1. Calls SCRCIN to inject the source into the appropriate grid blocks.
- Calls TPPRT to write the discharge information to the appropriate output files.

- Calls XCHNG to simulate diffusion to and from the rock matrix, if the matrix diffusion model is being implemented.
- 4. Sums the atoms that are currently in the catcher blocks for each leg in the migration path, puts the sum into the first grid block of that leg, and sets the atoms contained in the catcher blocks to zero.

After transport is complete, TRNSPT rewinds the source rate file (unit 24) and prints the atom count summary to the output file (unit 6) if the user has opted for this to be printed in the input options.

3.2.35 TSPFAC(DT, D, B, LT, TDP)

Called From	n	Calls
TIMER		

Function TSPFAC is called from TIMER to estimate the mean time a particle spends as each isotope over a time step for chains of five members or less. TSPFAC uses a Taylor series to calculate the Bateman coefficients that are needed to estimate this mean time.

3.2.36 WORK(IPASS, JTRIAL)

Called	From	Calla
NEF		SIFT

WORK is called from NEF after the transport simulation has been completed and performs several different functions. Initially, WORK condenses the temporary output arrays to account for non-transported decay chains, computes the weighted integrated discharges for each isotope, and prints an optional discharge summary for all of the isotopes to the hardcopy output file (unit 6) if the user requests this on input.

The remaining function of WORK is to write discharge rates to the discharge rate file (unit 30) based on the temporary files (unit 15 - 19, one file for each chain being transported) written by TPPRT, if the user has requested this output file to be written in the input options. The user may also request on input for all the isotope discharge rates to be written to the discharge file on the same time scale. Different time sc.les may arise because different DVM transport time steps are allowed for each different radioactive decay chain. To put all of the rates on the same time scale, WORK develops a general time scale based on the first minimum breakthrough time for all the isotopes and the simulation time. WORK appends the peak times and the simulation time to this general time scale and calls SIFT to sort the times into ascending order. WORK consolidates the sequence by accounting for ties and eliminates times exceeding the problem simulation time. WORK linearly interpolates times and the logarithm of the discharge rates from the temporary discharge files to find the discharge rates at the general time scale times.

3,2.37 XCHNG

Called From TRNSPT

XCHNG is called from the DVM transport model routine, TRSNPT, to implement the matrix diffusion model contained in NEFTRAN II, if the user has designated a leg as a dual porosity leg. Subroutine XCHNG is called at the end of each time step by TRNSPT to update the concentrations because of exchange with the matrix (i.e., immobile phase). The exchange is accomplished with a simple, linear mass-transfer equation and the concentration gradient is not allowed to change sign over a time step. XCHNG updates the concentration in the matrix caused by decay and production for the next time step.

Calls

3.3 Parameter Statements

The include file (SIZES.INC) required by NEFTRAN II stores the set of PARAMETER statements that define the dimensions of the arrays used in the code. If the user needs to change the dimensions of the arrays, only the PARAMETER statements have to be changed in the include file. These parameter statements are listed below along with definitions of each dimension parameter used by NEFTRAN II.

PARAMETER (MXLEG=25, MXJCT=25, MXLJ=5, NULCD=5)
PARAMETER (MXMEM=10, MXCHNS=6, MXPTH=10, MXNVI=7)
PARAMETER (MXGRD=1000, NDDF=2500, NDSF=2500)
PARAMETER (NDJPN=2000, NDBF=6000, MXELEM=30)
PARAMETER (MXTDV=20, MXQSC=100)
PARAMETER (MXISO=MXMEM*MXCHNS)
PARAMETER (MXISO=MXMEM*MXCHNS)
PARAMETER (MXSUB=(MXMEM*(MXMEM+1))/2)
PARAMETER (MXTSP=(MXMEM*(MXMEM+1))/2)
PARAMETER (MBDIM=MXSUB-MXMEM+1)*(MXMEM+2))/6-MXMEM)
PARAMETER (IBFDM=(MBDIM-1)*(MXPTH-1)*2)

MALEG	-01	The maximum number of legs for the flow network
MXJCT	*	The maximum number of junctions for the flow network
MXLJ		The maximum number of legs entering or exiting any junction
NULCD		The maximum absolute difference between connected junction
		numbers (Does not apply to junctions with known pressures)
MXMEM	*	The maximum number of isotopes per decay chain
MXCHNS	*	The maximum number of decay chains
MXPTH		The maximum number of legs in the migration path
MXNVI		The maximum number of intervals for velocity distribution
MXGRD		The maximum number of grid blocks
NDDF	*	The maximum dimension of the discharge-factor array
NDSF		The maximum dimension of the source-distribution array
NDJPN		The maximum dimension of the leg-transfer pointer array
NDBF		The maximum dimension of the leg-transfer fractions array
MXELEM	*	The maximum number of elements
MXTDV		The maximum number of time frames allowed to simulate time.
		dependent velocity fields
MXQSC		The maximum number of times allowed to simulate time-
		dependent flow through the source regime

The remaining PARAMETERS are functions of the above list and are defined as:

MXISC - The maximum total number of isotopes MXSUB - The maximum number of production subchains per chain MXTSP - The maximum dimension of the average time spent array MBDIM - The maximum number of subchains of length > { IBFDM - The maximum row dimension of the adjustment arrays

3.4 Common Blocks

All common blocks in NEFTRAN II are labeled and contain most of the arrays that are used by the code. In addition, there are a few arrays specific to certain subroutines. The following lists each common block statement along with a brief description of the labeled common block, and the arrays and parameters contained in the block. This listing is in alphabetical order according to common block label name.

COMMON/ BFIX / MBFX(MBDIM), IEFX(IBFDM,2), ABFX(IBFDM,2)

This block is only used if the leg-to-leg transfer algorithm is invoked. In that case, negative velocities can cause double counting of some particles. This is corrected by applying the correction fractions stored here. All fractions are calculated in subroutine ADJB and are applied in subroutine TRNSPT. The name BFIX arises from the notion that the atoms/ block calculated by the B-ARRAY are being fixed.

- MBFX MBFX(I) points to adjustment-fraction block numbers in the IBFX array for production subchain I. It is set in FACER and used in TRNSPT. In particular, contributor and receiver block indices that require correction for production subchain I are stored from IBFX(MBFX(I)+1,*) to IBFX(MBFX(I+1),*).
- IBFX Column 1 is a contributor block and 2 is a receiver block index that require correction for each production subchain. It is found in ADJB, printed in FACER, and used in TRNSPT.
- ABFX As part of calculating transport, TRNSPT applies the correction fraction in column 1 of ABFX to the contents of block IBFX(,1) and adds the product to block ABS(IBFX(,2)). If IBFX(,2) > 0, TRNSPT applies column 2 to the contents of IBFX(,1) and adds the product to block IBFX(,2) + 1. ABFX is found in ADJB and is printed in FACER.

COMMON/ DENSER / PEAK(MXISO), TIMPK(MXISO), TOTD(MXISO), 1 TIMBRK(MXISO), DWT(MXISO), WDIS(MXISO), WDISUM, NONZ

The name DENSER arises from the original intent of these arrays, to be used in condensing discharge rates in NEFTRAN (for a description see Longsine and others, 1987). In NEFTRAN II, condensing discharge rates has been replaced by the capability to place discharge rates from different chains on the same time gridding.

PEAK	. Peak discharge rates for each isotope (Ci/y), initialized in
	NEF, found in TPPRT, used and printed in WORK.
TIMPK	- Time of occurrence of the peak discharge rate (y), initialized in NEF, found in TPPRT, used and printed in WORK.
TOTD	- Total discharge for each isotope (Ci), initialized in NEF, found in TPPRT, used and printed in WORK.
TIMBRK	- Time of first nonzero discharge rate for each isotope (y), initialized in NEF, found in TPPRT, used in WORK.
DWT	- Total-discharge weighting factor for each isotope (/Ci), read in FLOWIN, printed in INPRIN, and applied in WORK.
WDIS	 Normalized total-discharge for each isotope, found and printed in WORK.
WDISUM	- Sum over all normalized discharges, found and printed in WORK.
NONZ	 Number of isotopes having nonzero discharge, initialized in NEF, found in TPPRT, used in WORK.
	COMMON/ FLOW / C(MXJCT), AW(MXJCT, 2*NULCD+1),

COMMON/ FLOW / C(MXJCT), AW(MXJCT, 2*NULCD+1), 1 JL(MXJCT, MXLJ), LJ(MXLEG, 2), JEQ(MXJCT), IB(MXJCT), 2 BCJ(MXJCT), NW, NL, NU, NB

This COMMON block contains information to set up and solve the flow network. The solution is cast as the matrix equation Ax = b. In the notation below, matrix A is called AW and both the constant (b) and solution (x) vectors are stored in array C.

- C In CUEFF, C is the constant vector containing the appropriate transmissibility-pressure products. In BSOLVE, C is converted to the calculated pressures, which are substituted into the pressure array, P of COMMGN JUNCT, by NEF.
- AW Banded matrix of transmissibilities, developed in COEFF and used in BSOLVE. Note that the bands are stored in rectangular form with each co-diagonal as a column.
- JL Legs connected to each junction, used to set off-diagonal entries in array AW by COEFF. Legs whose flow-direction is into the junction are labeled negatively and outflow legs are positive.
- LJ Junctions terminating each leg, read in FLOWIN, printed in INPRIN, used in COEFF, PTHLEN, and CHKPTH to develop the JL array and to reference junction properties.
- JEQ For each junction, stores its associated row index in the matrix equation (if the junction has unknown pressure) or zero (if the junction has known pressure) in COEFF. In NEFMAIN, JEQ is used to replace the solved pressures of vector C into vector P of COMMON JUNCT. Note also that this array is temporarily used in FLOWIN, STOPPER, and INFRIN to store and print junction pressure-boundary flags.
- IB Junction numbers having user-specified pressures, developed in FLOWIN and used in COEFF.
- BCJ Known pressures for the junctions stored in array IB (lb/ft²), developed in FLOWIN and used in COEFF.
- NW Number of rows of matrix AW and vector C, determined in COEFF and used in BSOLVE.
- NL Number of lower codiagonals of matrix AW, determined in COEFF and used in BSOLVE.

NU - Number of upper codiagonals of matrix AW, determined in COEFF.
 NB - Number of junctions with user-specified pressures, developed in FLOWIN and used in COEFF and NEF.

COMMON/ INAME / ISONAM(MXMFM), NAMALL(MXISO) CHARACTER*6 ISONAM, NAMALL

Isotope names are stored in the arrays of this common block. Each occurrence of this block is accompanied by the CHARACTER declaration shown. As evident from the CHARACTER declaration, isotope names can be no more than 6 characters.

- ISONAM Isotope names for the chain being transported, set in CHAIN from the NAMALL array and used for printing in subroutines BAND, SETUP, and TRNSPT.
- NAMALL Isotope names for all isotopes, read in FLOWIN, used in CHAIN, and used for printing in INPRIN, SOURCE, and WORK.

COMMON/ ISOTOP / CUROUT(MXMEM), LAMBDA(MXMEM), THALF(MXMEM), 1 VELISO(MXPTH,MXMEM), CI2ATM(MXMEM), IFR(MXMEM), BRFR(MXMEM), 2 NOISO, HLFALL(MXISO), LMTX(MXISO), CURALL(MXISO), 3 IPRALL(MXISO,2), FPRALL(MXISO,2), TRAVT(MXISO), NI(MXCHNS), 4 INCHN(MXCHNS), NCHNS, NTOT, MFNDX, ICH

This common contains information for all isotopes (dimensioned by MXISO) in all chains (dimensioned by MXCHNS) and has arrays designated for storing data for the current chain being transported (dimensioned by MXMEM). On input, all decay chain data are read, but following the printing of these data in INPRIN, FLOWIN compacts all arrays dimensioned by MXISO and MXCHNS to include only those chains marked for inclusion in source calculations. The descriptions that follow are pertinent for both data input (through printing) and compacted arrays (for subsequent use). Each occurrence of this common block is accompanied by type statement that declares variable LAMBDA as DOUBLE PRECISION.

- CUROUT Discharge rates for each isotope of the chain being transported at the current time (Ci/y), initialized to zero in METHOD, calculated for each time step in BAND and TRNSPT in atoms/y, and converted and printed in TPPRT.
- LAMBDA Decay constants for each isotope of the chain being transported (1/y), set to ln(2)/THALF in CHAIN, used in BRANCH, DTUPDT, SETDIS, MXCLL, TIMER, and BAND. Several other routines use the values in LAMBDA, but the values are passed to these routines via the calling sequence, usually in array D (which is also declared as DOUBLE PRECISION).
- THALF Half-lives for each isotope of the chain being transported (y), set from the HLFALL array in subroutine CHAIN and used in CHAIN and DXDT.
- VELISO Retarded velocities in each migration path leg for each isotope of the chain being transported (ft/y), found and stored in TRACER for steady-state flow runs. For time-dependent flow runs, VELISO is over-written for each time interval in TRACER. For each time interval, including a steady-state frame, TRACER

provides VELISO to DXDT to find space/time gridding for the time frame In METHOD, either the steady-state VELISO is used or VELISO is re-computed for each time frame. In either case, VELISO is then used in BAND and SETUP.

- CI2ATM Factors used to convert Curies to atoms for each isotope of the chain being transported (atoms/Ci), calculated in CHAIN as 1.6834x10¹⁸ x THALF and used in BAND and TPPRT. This conversion also occurs in the SOURCE routine, although CI2ATM is not explicitly used there.
- IFR A daughter indicator for each isotope of the chain being transported, developed in DTUPDT and over-written then redeveloped in CHAIN for use in BRANCH, SETDIS, MXCLL, and TIMER. For each isotope I, IFR(I) = 0 unless isotope I splits its deray to two daughters, in which case IFR(I) is the index of the first daughter encountered.
- BRFR A branching fraction for each isotope of the chain being transported, developed in DTUPDT and over-written then redeveloped in CHAIN for use in BRANCH, SETDIS, MXCLL, and TIMER. BRFR(I) = 0, unless IFR(I) = 0, in which case BRFR(I) is the branching fraction from parent I to daughter IFR(I). Note that the fractions in BRFR are subtracted from one and sent via calling sequence to several supporting routines, usually in array BFR.
- NOISO Number of isotopes in the chain being transported, used as a local variable and over-written in STOPPER, SOURCE, and DTUPDT, and set for decay chain transport in CHAIN from the NI arroy. The value set in CHAIN is used in DXDT, BRANCH, SETUP, SETDIS, FACER, MXCLL, TIMER, METHOD, BAND, TPPRT, TRNSPT, SRCIN, and XCHNG.
- HLFALL Half-lives for all isotopes (y), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in SOURCE, CHAIN, and DTUPDT.
- LMTX Element index for all isotopes, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in SOURCE and CHAIN to assign solubilities and retardations, respectively.
- CURALL Initial inventories for all isotopes (Ci), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in SOURCE.
- IPRALL Parent identifiers for all isotopes, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in CHAIN, BRANCH, and DTUPDT.
- FPRALL Branching fractions for all isotopes, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in CHAIN and DTUPDT.
- TRAVT Mean travel time for all isotopes (y), set in CHAIN by calling TRACER and used in DTUPDT and DXDT. There are two cases where TRAVT is set to an arbitrarily large number for an isotope by CHAIN - (1) if the isotope is in a decay chain that is included in source calculations but not transported and (2) if, for a time-dependent velocity run, the isotope cannot reach the discharge point in the total time simulated.
- NI Number of isotopes per chain, read in FLOWIN, checked in STOPPER, and used in SOURCE, CHAIN, DTUPDT, TRNSPT, WORK, and INPRIN.

INCHN . Inclusion flag for each chain, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in NEF, SOURCE, CHAIN, TRNSPT, and WORK. On input, each entry can be 0, 1, or 2. However, as stated above, all information for chains not included (2) is discarded, and the only values of INCHN then possible are 0 (source and transport) or 1 (source only).

NCHNS - Number of chains for source calculations, calculated in FLOWIN, checked in STOPPER, and used in NEF, SOURCE, DTUPDT, and WORK.

- Total number of isotopes for source calculations, calculated in NTOT FLOWIN and used in SOURCE, DTUPDT, and WORK.
- MFNDX Cumulative number of isotopes to the end of the previous chain, 10 calculated and over-written in SOURCE, DTUPD'r, and WORK and determined for transport of each chain in CHAIN. The latter value is then used to reference arrays in BRANCH, DXDT, and TPPRT.
- ICH Index of the chain being transported, set and over-written in SOURCE, DTUPDT, and WORK and set for transport of each chain in NEFMAIN. The latter value is then used to reference arrays and disc file unit numbers in CHAIN, METHOD, TPPRT, and TRNSPT.

COMMON/ JUNCT / P(MXJCT), EL(MXJCT)

This block contains all junction properties, with the exception of the boundary conditions found in COMMON FLOW (IB, BCJ, and NB).

P - Pressures at all junctions (1b/ft2). In FLOWIN, P is used to temporarily store the user-specified boundary pressures (in psi units) and is zeroed out after being used to print the input pressures in INPRIN. In COEFF, the boundary pressures (converted from psi to 1b/ft2 in FLOWIN and stored in array BCJ, see COMMON FLOW) are placed into the appropriate locations in the P array. In NEFMAIN, the calculated pressures (see array C, COMMON FLOW) are slotted into the remaining locations. Subroutine PTHLEN uses the pressures in P to calculate flow rates for each leg and optionally prints P in input units, psi. EL - Elevations for each junction (ft), read in FLOWIN, printed in INPRIN, and used in COEFF and PTHLEN.

COMMON/ LEGS / AREA(MXLEG), BC(MXLEG), COND(MXLEG), Q(MXLEG), 1 FDENS(MXLEG), PATH(MXLEG), TH(MXLEG)

The leg properties stored here relate to the flow network, so each array is dimensioned to the maximum number of network legs, as opposed to leg properties specific to the migration path which are stored in COMMON MISC, discussed below. If the flow network is not solved, the only array used from this block is the leg-lengths array, PATH.

AREA - Cross-sectional area perpendicular to flow for each leg (ft²), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in COEFF and PTHLEN.

 Relative brine concentration for each leg (dimensionless between 0 and 1), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in COEFF.

COND - Hydraulic conductivity for each leg (ft/y), read in FLOWIN in units ft/day, printed in INFRIN, and then converted in FLOWIN to ft/y for use in COEFF.

BC

0

TH

- Volumetric fluid flow rate through each leg (ft³/y), calculated in PTHLEN and checked in CHKPTH. Note, if velocities are input directly, Q is equated to velocity in each leg prior to the call to CHKPTH for checking flow directions.
- FDENS Fluid density of each leg (lb/ft³), calculated in COEFF and used in PTHLEN.
- PATH Length of each leg (ft), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in COEFF, PTHLEN, TRACER, CHAIN, SETUP, FACER, and DXDT.

- Transmissibility for each leg (mixed units), calculated and used in COEFF and used again in PTHLEN.

COMMON/ MISC / ALPHA(MXPTH), PHI(MXPTH), PORE(MXPTH), DXDTPA(9), 1 DTCHN(MXCHNS), DT, Y, MPATH(MXPTH), LCH MXC, LTOLX, IXCHG, 2 NELM, NLEG, NJCT, NPATH

As the name MISCellaneous suggests, this is somewhat of a catchell common block. Migration path properties and the time step are the most often used variables listed here.

- ALPHA Dispersivities for each leg in the migration path (ft), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in UXDT, BAND, and SETUP. For the analytical solution transport model and for path-averaged-DVM transport using leg-averaged velocities, only one value of dispersivity is used. It is taken to be the first value of the array, ALPHA(1).
- PHI Mobile phase porosity for each leg in the migration path, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in PTHLEN to convert steady-state Darcy flux to pore velocity and in XCHNG to compute mobile phase concentrations.
- PORE Steady-state pore velocity for each leg in the migration path (ft/y), read in FLOWIN and, if the flow network is solved, over-written in PTHLEN. PORE is checked in STOPPER, printed in INPRIN, and used in TRACER and CHAIN.

DXDTPA - Increment-determination parameters for the DVM transport model, read or defaulted in FLOWIN and used in DXDT.

- DTCHN DTCHN(I) is the user-specified time step for the transport of decay chain I, read in FLOWIN, printed in INPRIN, and used in CHAIN. If input as zero, DXDT determines a time step for that chain. Note that for time-dependent velocity runs, the userspecified value may be modified so that there is an integer number of time steps for each time interval.
- DT Current time step for source or transport (y). If provided by the user, DT for source is equated to DTSRC in DTUPDT. DT for the DVM transport model is equated to DTCHN(I), for each chain I, in CHAIN and DT is calculated in METHOD if the analytical

solution transport model is chosen. Since the time step for transport can change for the time intervals specified by timedependent velocity data, accepted values of DT for each time frame (determined in DXDT) are stored in the TDDT array of COMMON VELFLD, for retrieval by routine METHOD. The source DT is used by SOURCE, BRANCH, and DTUPDT. The transport DT is used by CHAIN, DXDT, SETUP, BRANCH, TIMER, MXCLL, SETDIS, METHOD, BAND, TPPRT, TRNSPT, SRCIN, and XJHNC. There is one other use for DT. DT is temporarily set to release time (TRLSE, see COMMON OUTVC) by subroutine SOURCE prior to calling BRANCH, in order to update the inventories to TRLSE.

 Distance from the leading edge of the source regime to the discharge boundary (ft), computed by adding leg lengths in PTHLEN. Y is reported in PTHLEN and used in TRACER, CHAIN, DXDT, SETUP, METHOD, and BAND.

- MPATH Migration path leg indices, read in FLOWIN checked in STOPPER, printed in INPRIN, and used in PTHLEN, CHKPTH, TRACER, CHAIN, DXDT, SETUP, and FACER.
- LCH Source model flag: (0) leaching only, (1) solubilities only, or (2) both are considered in finding source rates. Set in STOPPER to option 19 and used in FLOWIN and DTUPDT.
- MXC Source model flag: (0) fluid flow-through, (1) fluid dilution as modeled by a mixing cell, or (2) let code choose between 0 and 1 to distribute source rates into transport path. Set in STOPPER to option 20 1.1 used in FLOWIN.
- LTDLX A DVM transport flag; (0) leg-averaged velocities or (1) the leg-to-leg transfer algorithm will be used to transport radionuclides. LTOLX is set in FLOWIN to option 22, but may be over-written if option 22 is zero and matrix diffusion is to te modeled or time-dependent flow fields are input. LTOLX is used in CHAIN, DXDT, SETUP, METHOD, and TRNSPT.
- IXCHG A DVM transport flag; (0) no matrix diffusion or (1) yes matrix diffusion will be included for transport. IXCHG is set in FLOWIN after reading the migration path properties, in particular, the leg-dependent diffusion flags. IXCHG is used in STOPPER and TRNSPT.
- NLEG Number of legs in the flow network, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in COEFF and PTHLEN.
- NJCT Number of junctions in the flow network, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in NEF, COFFF, and PTHLEN.
- NPATH Number of legs in the migration path, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in PTHLEN, CHKPTH, TRACER, CHAIN, DXDT, SETUP, SETPIS, METHOD, and XCUNG.

COMMON/ OPTION / IOPT(38)

Y

The intent of individual options is described in Section 4.3.1, so only the definition and use of the entire erray is mentioned here.

IOPT - Options, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in NEFMAIN, FLOWIN, STOPPER, INPRIN, COEFF, PTHLEN, TRACER, SOURCE, CHAIN, DTUPDT, DXDT, SETUP, TIMER, FACER. MXCLL, SETDIS, METHOD, BAND, GIT, TPPRT, TRNSPT, WORK, and GETRV.

COMMON/ OUTVC / TUB, TRISE, 7LCH, SUMIN(MXMEM), SUMOUT(MXMEM), 1 ICOUNT, IFREQ, QDAREA, OUIS

This common block (OUTVC) contains some output controls and summary information.

- TUB Problem simulation time (y), read in FLOWIN, printed in INPRIN, and used in NEFMAIN, PTHLEN, TRACER, SOURCE, CHAIN, DTUPDT, METHOD, TPFRT, and WORK.
- TRLSE Time of initial radionuclide-fluid certact (y), read in FLOWIS, checked in STOPPER, printed in INPRIN, and used in PTKLIN, TRACER, SOURCE, CHAIN, DTUPDT, DXDT, METHOD, TPPRT, TRNSPT, and SRCIN.
- TLCH Time of onset of leaching (y), read in FLOWIN, checked in STOPPER, printed in INFRIN, and used in SOURCE and LECHMOD.
- SUMIN Total amount input as source for DVM transport for each isotope (atoms), zeroed-out in METHOD, accumulated in SRCIN, and reported in TRNSPT.
- SUMOUT Total amount discharged from DVM transport for each isotope (atoms), zeroed-out in METHOD, accumulated and reported in TRNSPT.
- ICOUNT Time step counter for frequency of printing discharge rates to hardcopy output file (unit 6), initialized in METHOD (for DVM) and BAND (for analytic solution) and used and reset in TPPRT.
- IFREQ Discharge rates are printed to the hardcopy output file (unit 6) every IFREQ time steps. IFREQ is set to the absolute value of option 19 in FLOWIN and is used in METHOD, SAND, AND TEPRT.
- QDAREA Product of cross-sectional area perpendicular to flow and porosity, at the discharge point (ft²), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used to calculate QDIS, below, in PTHLEN and METHOD.
- QDIS Flowrate at discharge (ft³/y), either set to the calculated flowrate of the last leg in the migration path by PTHLEN or, if the network is not solved, is set to the product of QDAREA and the pore velocity of the last leg in the gigration path by PTHLEN (steady-state runs) or METHOD (time-dependent flow runs). QDIS is used in TPPRT to convert radionuclide discharge rates to concentrations.

COMMON/ QSOURCE / TSRCE(MXQSC), QSRCE(MXQSC) NQSC

This common contains information to simulate a time-varying flowrate through the source regime. There can be fixed flow (in which case none of the data here is required) or time-varying flow for steaky-state runs. However, runs using time-dependent velocities automatically generate time-varying source flowrates, if not input explicitly designated by the user. TSRCE - TSRCE(1) is the time to which flowr, to QS 2(1) applies (y), Fig. , either road in FOWIN from an external file (see Section 4.3.1) is set in FLOWIN if the time frames specified for the the a condent velocities given in TDTM of COMMON VELFLD. THAVE is becked in STOPPER, printed in INPRIN, and used in SCURCE AND MURDT.

QSFCF -

QARCE(1) is the flowrate through the source regime which applies to thme TSRCE(1) (ft³/y), and is either read in FLOWIN from an enternal file or calculated in FLOWIN as the product of the time dependent pore velocities given in the first column of TDVEL of COMMON VELFLD and QSAREA of COMMON SOLIMT. QSRCE is checked in STUPPER, printed in IMPRIN, and used in SOURCE and DTUPDT .

NOSC

Number of times specified for simulating time-dependent flow t) rough the source regime, set in FLOWIN (upon encountering an end-of-file marker or set to MFL2 of COMMON VELFLD if the timedependent velocities were used) and used in INPRIN, SOURCE, and DTUPDT .

COMMON/ RETARD / AKI(MXPTH, MXELEM), AKIM(MXPTH, MXELEM), 1 RKI(MXPTH, MXMEM), RKIM(MXPTH, MXMIM)

The retardation factors for both the mobile and immobile phases are stored here by eleven, and leg for all elements and by isolove and leg for the isotopes of the chain being transported.

- Retardation factors in the mobile phase for each migration leg AKI and each element, read in FLOWIN, checked in STOPPER, printed 'n IMPRIM, and used in CHAIN.
- AKIM Retardat on facto; s in the immobile phase for each migration leg and each element, read in FLOWIN, checked in STOPPER, printed in INPRIM, and used in CHAIN.
- RKI Petardation factors 10 the modifie phase for each migration leg and each isotope in the chain being transported, set in CHAIN and used in CHAIN, TRACER, METHOD, and XCHNG,
- R/IM Retardation, factors in the immobile phase for each migration leg and each isotope in the chain being transported, set in CHAIN and used in XCHNG.

COMMON/ SOLIMI / CSALL(MEAGLEM), AMALL(MEASO), DTPAR(7), ACSSFR, 1 LLONL , IDSRG, VOL, QSAREA, QSC, LMODEL, RLCH, SAL, DTSRC

Most of the information required for source calculations is included in this common block.

- Solubility limit for each element (g-element/g-fluid), read in FLOWIN, chucken in STOPPER, printed in INPRIN, and used in SOURCE.
- AMALL
- Atomic mass for each isotope, read in FLOWIN, checked in STOPPER, privated in INPFIN, and used in SOURCE.

- DTPAR Source time-step determination parameters, read or defaulted in FLOWIN and used in DTUPDT
- ACSSFR Fraction of the inventories input in CURALL of COMMON IS TOP to be used for source calculations, read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in SOURCE and BAND.
- LLONLY Source control parameter which is assigned one of the first six values of IDSRC (below) following the mixing cell ferribility check, set in DTUPDT and used in SOURCE, SETUP, and SPLIN.
- IDSRC Source control parameter for leach/solubility and mixing cell, set to 3(MXC) + LCH (see COMMON MISC) by FLOWIN and used in DTUPDT.
- VOL Fore volume of the source regime for mixing cell calculations (ft³), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in SOURCE and DTUPDT.
- QSAREA Product of cross-sectional area perpe.Jicular to flow and porosity of the source regime (ft²), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used to calculate QSC, below, in PTHLEN and to calculate QSRCE of COMMON QSOURCE in FLOWIN.
 - SC Fluid flow rate through the source regime (ft³/y). For steadystate source-flow runs, QSC is set in PTHLEN to the calculated flow rate of the first leg in the migration path (if the flow network is solved) or to the product of QSAREA and the pore velocity of the first leg in the migration path (if the flow network is not solved). For time-dependent runs, QSC is set to the flow rate in QSRCE of COMMON QSOURCE that corresponds to the appropriate time interval. QSC is used in SOURCE and DTUPDT.
- LMODEL A leach model flag; (0) constant leach rate or (1) exponential leach rate is used in finding source rates. Set in STOPPER to option 21 and used in LECHMOD.
- RLCH Leach rate for the specified leach model (1/y), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in DTUPDT, LECHMOD, and BAND.
- SAL Fluid density in the source regime (lb/ft³), read in FLOWIN, checked in STOPPER, and printed in INPRIN. If the flow network is solved, SAL is replaced in PTHLEN by the fluid density calculated for the first leg in the migration path. SAL is used in SOURCE.
- DTSRC User-specified time step for source calculations (y), read in FLOWIN, printed in INPRIN, and checked and used in DTUPDT. If specified as zero, DTUPDT determines the time step.

COMMGN/ VELFLP / TDTM(MXTDV), TDVEL(MXTDV,MXPTH), 1 TDSAT(MXTDV,MXPTH), TDDT(MXTDV), MFL1, MFL2

Data to simulate time-dependent velocity fields is included in this common block.

TDTM - TDTM(I) is the time to which the velocities TDVEL(I,MXPTH) apply (y), read in FLOWIN from an external file, checked in STOPPER, and printed in INPRIN. TDTM is used in FLOWIN to set TSRCE of COMMON QSOURCE (if TSRCE is not specified). TDTM is also used in TRACER, CHAIN, and METHOD. For steady-state runs, TDTM(1) is set to TUB of CGAMON OUTVC by FLOWIN and only the first entry is referenced.

TDVEL +

DX

TDVEL(I,J) is the pore fluid velocity for the Jth leg in the migration path that applies to time TDTM(1) (ft/y), read in FLOWIN from an external file, checked in STOPPER, and printed in INPRIN. TDVEL(I,1) is used in FLOWIN with QSAREA of COMMON SOLIMT to calculate QSRCE of COMMON QSOURCE, if QSRCE is not specified. TDVEL is also used in PTHLEN, TRACER, CHAIN, and METHOD. For steady-state runs, TDVEL(1,J) is set to PORE(J) of COMMON MISC by PTHLEN and only the first time entry is referenced.

TDSAT - TDSAT(I,J) is the saturation for the Jth leg in the migration path that applies to time TDTM(I), read in FLOWIN from an external file, checked in STOPPER, and printed 'n INFRIN. TD:AT is used in TRACER and METHOD. For steady-state runs, TDSAT(1,J) is set to one for all migration legs by PTHLEN and only the first time entry 14 referenced.

TDDT - TDDT(I) is the time step for the chain being transported for time frame 1 (y), set in CHAIN follow: 3 the call to DXDT, and retrieved by METHOD. For steady-state runs, TDDT(1) is set to DT of COMMON MISC by CHAIN following a call to DXDT and only the first entry is referenced.
MFL1 - Smallest index in TDTM such that time TDTM(MELL) is at least to

 Smallest index in TDTM such that time TDTM(MFL1) is at least as large as release time, TRLSE of COMMON OUTVC. MFL1 is found in STOPPER, but is set to one by FLOWIN for steady-state runs.
 MFL1 is used in PTHLEN, TRACER, CHAIN, and METHOD.

MFL2 - Smallest index in TDTM such that time TDTM(MFL2) is at least as large as simulation time, TUB of COMMON OUTVC. MFL2 is found in STOPPER, but is set to one by FLOWIN for steady-state runs. MFL2 is used in PTHLEN, TRACER, CHAIN, and METHOD.

COMMON/ XFER / NX(MXPTH), NC(MXPTH), DX(MXPTH), TMN(MXTSP), 1 BF(NDBF), JFSC(MXSUB+1), JPN(NDJPN,3), IMB(MXPTH), 2 PHIM(MXPTH), XFC(MXPTH), JBF(MXMEM)

Data for the leg-to-leg transfer algorithm is stored in this block, along with matrix diffusion data. If path-averaged velocities are used, only the first entries of NX, NC, and DX are required.

- NX Number of grid blocks for each leg in the migration path, determined in DXDT and possibly refined in CHAIN. NX is used in SETUP, FACER, TRNSPT, and XCHNG.
 Number of catcher blocks for each leg in the migration of catcher blocks.
 - Number of catcher blocks for each leg in the migration path, determined in DXDT and possibly refined in CHA'N. NC is used in FACER, TRNSPT, and XCHNG.
 - Grid block size for each leg in the migration p th (ft), read in FLOWIN and printed in INPRIN. Nonzero DX is checked in DXDT, otherwise, DX is determined in DXDT. Code-determined DX is potentially refined in CHAIN due to dimensioning and in SETUP to preserve the length of each leg. DX is used in FACER, ADJB, MXCLL, and SETDIS. Note that DX(1) and DXX of COMMON XPORTB are identical for path-averaged velocity runs.

- TMN Mean time spent over a transport time step as each isotope in each production subchain (y), determined and printed in TIMER and used in SETUP and FACER.
- BF Transfer fractions for particles crossing into new legs over a transport time step, determined and printed in FACER and applied in TRNSPT.
- JPSC Pointers to blocks of data in JPN array, below, for each subchain. That is, for subchain I, all contributor and receiver block indicies for leg-to-leg transfer are found between entries JPN(JPSC(1)+1) and JPN(JPSC(1+1)), where JPSC(1) = 0. JPSC is found and printed in FACER and used in TRNSPT.
- JPN Receiver and contributor block indicies from the log-to-leg transfer algorithm. Block JPN(I,1) is contributed to over a time step from blocks JPN(1,2) to JPN(1,3), although with large Courant numbers there may be blocks in between these latter two indicies that do not contribute. JPN is determined and printed in FACER and used in TRNSPT.
- IMB Flag indicating presence (1) or not (0) of an immobile phase for each leg in the migration path, read in FLOWIN and printed in INPRIN. IMB is used in STOPPER, CHAIN, and XCHNG.
- FHIM Porosity in the immobile phase for each leg in the migration path, read in FLOWIN, checked in STOFFER, printed in INPRIN. and used in XCHNG.
- XFC Mass-transfer rates for each leg in the migration path (1/y), read in FLOWIN, checked in STOPPER, printed in INPRIN, and used in XCHNG.
- JBF JBF(1) is the index of the first transfer fraction in the BF array for subchains ending in isotope 1. JPF is found in FACER and used in TRNSPT.

COMMON/ XPORTA / RHO(MXGRD,MXMEM), RHONEW(MXGRD), F(NDDF), 1 SF(NDsF), RHOM(MXGRD,MXMEM)

This common contains several of the large chain- and grid-dependent arrays for the DVM transport model.

- RHO Amount (atoms) in the mobile phase for each grid block and for each isotope being transported, initialized to zero in METHOD and updated for each time step in TRNSPT, SRCIN, and XCHNG. Also used in TRNSPT for discharge calculations and atom count summaries.
- ***ONEW Amount in the mobile phase for each grid block for a specific isotope being transported (atoms), initialized to zero in METHOD and used for temporary storage while updating the RHO array, above, in TRNSPT.
- F Discharge fractions over a transport time step for each subchain, found and printed in SETDIS and used in TRNSPT.
- SF Source distribution fractions over a transport time step for bach subchain, found and printed in MXCLL and used in SRCIN.

RHOM - Amount in the immobile phase for each grid block and for each isotope being transported (atoms), initialized to zero in METHOD and updated for each time step in XCHNG. Also used in TRNSPT for computing atom count summaries.

COMMON/ XPORTE / B(2*MXNVI, MXSUB, MXPTH), JV(2*MXNVI, MXSUE, MXPTH), 1 V(MXNVI, MXSUB, MXPTH), DF(MXSUB), N(MXSUB, MXPTH), JF(MXSUB+1), 2 LPS(MXMEM), LPE(MXMEM), LRF(MXSUB,2), JSF(MXSUB+1), INSR(MXSUB), 3 DXX, INSRC, KFDT, KFDX(MXPTH), KFDXA, NSE, NTX, NVI

This common contains mostly arrays stacked by subchain for the DVM transport model.

B

JV

V

DP

N

JF

LPS

 Transport fractions for each subchain being transported for particles that remain in a leg over a transport time step, found and printed in SETUP and used in TRNSPT.

- Pointers to the transport fractions in array B, above, for each subchain being transported for particles that remain in a leg over a transport time step, found and printed in SETUP and used in TRNSPT. In particular, for subchain J in leg K, block I receives contribution from blocks 1 - JV(L,J,K) over a time step, where L = 1, ..., N(J,K) (see N below). The fractions of the contributor blocks that wind up in block I are found in B(L,J,K), where L = 1, ..., N(J,K). Note that K is set to one for path-averaged velocity runs.

Distributed velocities for each subchain being transported for each leg in the migration path (ft/y), found, used, and partially printed in SETUP and used in FACER, MXCLL, and SETDIS. In particular, V(I,J,K) is the Ith velocity for subchain J in leg K. Note that K is set to one for path-averaged velocity runs.

 Decay survival fractions and production fractions over DT for each subchain. Here, DT, as described in COMMON MISC, can be TRLSE of COMMON OUTVEC, the time step for source calculations, or the time step for DVM transport calculations. DP is found in BPANCH using FUNCTION ET and is printed in SETUP, when DT is the transport time step. DP is used in SOURCE, DTUPDT, SETUP, TIMER, FACER, ADJB, and XCHNG.

- Number of contributor blocks to any interior block in each lrg of the migration path for each subchain being transported, found and printed in SETUP and used in TRNSPT. In particular. N(J,K) is the number of contributor blocks in leg K for p.o. chain J. Note that K is set to one for path-averaged values/cy runs.
- Pointers to sets of fractions for each subchain in the discharge factor array, F of COMMON XPORTA, found in SETDIS and used in TRNSPT. In particular, the discharge fractions for subchain I are stored contiguously from F(JF(I)+1) to F(JF(I+1)).
- LPS(I) points to the beginning of subchain information for subchains ending with isotope I, found in BRANCH and used in DTUPDT, SETUP, TIMER, FACER, MXCLL, TRNSPT, SRCIN, and XCHNG.

For example, the decay survival fraction for isotope 1 over a time step is stored in DP(LPS(I)). LPS is also used as a locator for arrays B, JV, V, N, LRP, INSR, JF, and JSF described here and JPSC of COMMON XFER.

LPE(I) points to the end of subchain information for subchains ending with isotope I, found in BRANCH and used in DTUPDT, SETUP, TIMER, FACER, MXCLL, TRNSPT, SRCIN, and XCHNG. For example, the decay survival fraction for isotope I over a time step, followed by the production fractions for all subchains ending in isotope I, are stored from DP(LPS(I)) to DP(LPE(I)). LPE is also used as a locator for arrays B. JV. V. N. LRP. INSR, JF, and JSF described here and JPSC of COMMON XFER.

Parent and subchain length for each subchain being transported, found in BRANCH and used in DTUPDT, SETUP, TIMER, FACER, ADJB, MXCLL, TRNSPT, SRCIN, and XCHNG. For subchain 1, LRP(1,1) is the index of the first member of the subchain and LRP(1,2) is the number of isotopes in the subchain.

Pointers to sets of fractions for each subchain in the source distribution array, SF of COMMON XPORTA, found and printed in MXCLL and used in SRCIN. In particular, the source distribution fractions for subchain I are stored contiguously from SF(JSF(I)+1) to SF(JSF(I+1)).

INSR(I) is the number of grid blocks in the up-gradient direction to receive source for subchain I, found in MXCLL and used in SRCIN. INSR is only used for the mixing-cell source distribution scheme and is used in conjunction with INSRC, described below.

Grid block size for transport for runs that use leg-averaged velocities (ft), set to DX(1) by FLOWIN. Nonzero values are checked in DXDT, otherwise DXDT determines an appropriate value. Code-determined values of DXX may be further refined to preserve total path length in DXDT. DXX is used explicitly in MXCLL and implicitly as DX(1) in SETDIS.

INSRC Index of the first block to receive source for runs that use the fluid flowthrough source model, determined in SETU? and used in SRCIN. If the mixing cell source model is used, INSRC is the index of the first non-catcher block. Source distribution for subchain I therefore starts with block INSRC -INSR(I), where the latter array is described above.

- KFDT Flag indicating whether the user has specified (1) the transport time step for the decay chain being transported or not (0), set in CHAIN and used in DXDT.
- KFDX(I) is a flag indicating whether the user has specified (1) KFDX the transport space step for leg I of the transport path or not (0), set in FLOWIN and used in CHAIN, DXDT, and SETUP.
- Number of legs for which the user has specified the transport KFBXA space step, set in FLOWIN and used in CHAIN, DXDT, and SETUP.
 - Number of grid blocks to receive the source injection calculated using the flowthrough source model, set to NX(1) by SETUP if the leg-to-leg transfer algorithm is used and set to the ratio of the length of the first leg of the migration path to the grid block size DXX by DXDT if leg-averaged velocities are used. For runs that use the mixing cell source model, NSB is set to zero in SETUP. NSB is used by SRCIN.

LRP

LPE

.

JSF

INSR

DXX

- NTX Total number of grid blocks, determined in CHAIN following the final refinements of the space steps and the catcher blocks. NTX is used in FACER, TRNSPT, and XCHNG.
 - Number of intervals over which the isotope velocities are distributed, set to the first increment determination parameter by FLOWIN, either from user-specified input or from the default value 7. NVI is used in DXDT, SETUP, FACER, ADJB, and MXCLL.

NVI
4.0 DATA INPUT GUIDE

The data input guide is divided into six sections. Section 4.1 describes the execution procedure for NEFTRAN II. Section 4.2 describes, in general terms, both the parameters and arrays required in the NEFTRAN II input file. Section 4.3 and Section 4.4 provide detailed descriptions of parameter and array input, respectively. The specific units required for the input data are discussed in sections 4.3 and 4.4, but in general, the code requires data to be input in English Engineering System units. The input requirements for running multiple data sets are defined in Section 4.5 and a sample input file is discussed in Section 4.6.

4.1 Execution Procedure for NEFTRAN II

There are two versions of NEFTRAN II. The PC (personal computer) version has been compiled with Microsoft Fortran Version 2.3 and can be run on a personal computer. The PC memory requirements depend on the size of the arrays used by NEFTRAN II (see Section 3.3), which in turn, depends on the size of the problem being simulated.

To execute NEFTRAN II on a personal computer using the disk operating system (DOS), the user must type:

NEFII\Pathname\Filename

where "\Pathname\Filename" will be retrieved in subroutine FLOWIN and stored as a character string up to, but not including, the extension of "Filename." The character string (ROOT, used in FLOWIN and NEFMAIN) is then used to access other input files, if required, and to name output files as requested. Note that "Filename" need not have an extension, but it must be included on the command line if it does have an extension. Also, "\Pathname\" must be included only if "Filename" exists in a directory different from the one containing the executable file (NEFII.EXE).

This execution procedure allows the user to use any name for the NEFTRAN II input file(s) and also allows the user to execute NEFTRAN II from one directory and write/access input/output files to another directory. For example, suppose the input file name is TEST.INP and resides in the same directory as the executable (NEFII.EXE). Then to execute this input file, the user would type:

NEFII TEST. INP

("\Pathname\" is not needed since the input file and the executable reside in the same directory). The naming of the auxiliary files would proceed as follows:

On input (as required)

- TEST.VEL (unit 11) must be the name of the data file containing time-dependent velocity fields.
- TEST.QSC (unit 12) must be the name of the data file containing time-dependent flow rates through the source.

 TEST.SMP (unit 10) must be the name of the data file containing sampled data for over writing input.

On Output (as requested)

- TEST.OUT (unit 6) is the name of the hardcopy output file written by NEFTRAN II.
- 2. TEST.DIS (unit 30) is the name of the output file containing discharge rates written by NEFTRAN II.
- TEST.SRC (unit 25) is the name of the output file containing source rates written by NEFTRAN II.

This file naming scheme is useful for keeping track of input/output files that are required or generated by NEFTRAN II by ensuring consistency, and give the user a means of quality control.

For the VAX version of NEFTRAN 11, the standard VAX computer execution procedure is required (i.e., RUN NEFII). The main difference between the VAX version and the PC version is the file naming scheme. For the VAX version, the input file(s) must be named NEFII with the appropriate extension, instead of an arbitrary user input character string. For example, to run NEFTRAN 11 on the VAX, input must reside on a file named NEFII.INP. The auxiliary input files, as required, must be named NEFII.VEL, NEFII.QSC, and NEFII.SMP. The output files that NEFTRAN 11 would create, as required, would be named NEFII.OUT, NEFII.SRC, and NEFII.DIS. This required file naming procedure for the VAX version is equivalent to the PC version for ROOT equal to NEFII.INP. In the following discussion of input requirements, the name of the external files will be denoted (root) with the appropriate extension, in reference to the above PC version file naming scheme.

4.2 General Input Description

All read statements for the input file are found in subroutine FLOWIN. Following the read of the 60-character string title, five sets of parameter data and five arrays are required. For the five arrays to be read, an array title and the actual data are required. Each row of the array is read on a separate record. Every set of parameters and array has a number of error checks in subroutine STOPPER.

Except for the character data (title and array names), all read statements are list-directed. This helps avoid errors involving field width and alignment. However, because the read statements are list-directed, every parameter and array entry must be assigned a value. That is, use of a blank to indicate zero is not permissible. Currently there are up to 55 single-valued parameters that can be input to NEFTRAN II. Each parameter is read on a separate record. Using list-directed format, the value can be followed by a comma or blank and the rest of the record is ignored. If the user chooses to do so there is ample space to append a descriptive comment to each value. With this feature, and proper use of the array names, the input file can be generated in the form of a template. The use of a template allows the user to easily edit existing input files for data input changes and also minimizes references to a data input guide for a description of the input required. In sections 4.3, 4.4, and 4.5, for each set of data required, a sample input template is also provided.

If the user opts to include multiple data sets in a single simulation, the first record on the second and subsequent data sets contains flags indicating which of the ten input groups are to be read again. Since the title is not read again, the ten flags required consist of five flags for the parameter sets and five for the arrays. For array input, both the array names and array data must be supplied for all data sets. Data checking is also performed in STOPPER on the later data sets. Note that if external files are attached that contain supplemental input, they are re-wound and re-read for each data set, provided the option to use the file does not change.

4.3 Parameter Input Description

There are five sets of parameters that are input to NEFTRAN II. They include most of the options, dimension parameters, and physical parameters that appear in NEFTRAN II input file. Some parameters are derived from other input data. In particular, the option to implement the leg-to-leg transfer algorithm is automatically invoked if an external file of time-dependent velocities is used or if diffusion from mobile to immobile fluid occurs for any leg in the migration path. The latter criterion is used to decide whether the global diffusion flag is zero or nonzero. Also, two input parameters (LCH and MXC, described below) are used to determine an appropriate value for the source-type parameter IDSRC. The next five subsections describe the input for the five sets of parameter data.

4.3.1 Options

<u>Standard Print Options</u>. One dummy title record and 11 records of single integer data. The standard print options are flags that indicate whether NEFTRAN II will print certain information to the hardcopy output file ((root).out, unit 6). For each print option, zero means do not print and a nonzero integer implies print. The following discussion lists the information that is printed for each option. This information is considered standard in the sense that it is useful to the user when the code is executing without any problems. Note that options 2 - 6 echo the array input without any change of units.

Ontion	Output	Printed 1	f Option	is a Non	zero Integer
P. P. P. T. P. P. P.	Ser has been been been a	A . A. A. A. A. M. M. M.	and the second	And so when the second	the second states and the second states and the second states and the

- IOPT(1) The complete set of parameters.
- IOPT(2) The network leg properties array.
- IOPT(3) The network junction properties array.
- IOPT(4) The migration leg properties array.

- IGPT(5) The inventory array.
- IOPT(6) The element properties array.
- IOPT(7) Fluid velocities and source/discharge flow rates.
- IOPT(8) Subchains, production factors, and velocities, only relevant for the DVM transport model.
- IOPT(9) Space and time increments and source type, only relevant for the DVM transport model.
- IOPT(10) Time-dependent output at the discharge point. If positive (e.g., +N) then discharge rates (Ci/y) are printed every Nth time step. If negative (e.g., -N), concentrations (Ci/ft³) are printed every Nth time step.
- IOPT(11) Discharge summary (peak rates and integrated discharge).

An example of the template that can be used in the input file for these standard print options is given in Table 4.1.

External File Options. Ose dummy title record and six single value integer records. In NEFTMAN II, external files are used to either store results (i.e., write-to) or for supplemental input (i.e., read-from). Specifically, external files are (1) used to store resultant source rates and discharge rates, (2) can be used to provide data to subroutine GETRV to over write selected input, usually with statistically sampled data, and (3) can be used to input time-dependent velocity fields and

Table 4.1.

Input Template for Standard Frint Options

	PARAMETERS, GROUP1 - OPTIONS, STANDARD PRINT, NONZERO -> PRINT
0	LIST OF ALL PARAMETERS
0	THE NETWORK LEG PROPERTIES ARRAY
0	THE NETWORK JUNCTION PROPERTIES ARR Y
0	THE MIGRATION PATH PROPERTIES ARRAY
0	THE DECAY CHAIN PROPERTIES ARRAY
0	THE ELEMENT PROPERTIES ARRAY
0	FLUID VELOCITIES & SOURCE/DISCH FLOWS
0	SUBCHAINS, PRODUCTION & VELOCITIES
0	SPACE & TIME STEPS AND SOURCE TYPE
0	TIME DEPENDENT OUTPUT, IF +/-N, RATES/CONC3 EVERY NTH TIME STEP
0	DISCHARCE SUMMARY

time-dependent flow rates through the source regime. The following discussion will list each option and describe the external file that is either read-from or written-to. For all the external file options a zero implies not to write/read the external file and a nonzero integer indicates the opposite. The user should also note the added significance of the sign of option 13.

Option External File Description

- IOPT(12) If nonzero, write source rates to unit 25. Note, unit 25 is opened by the code with the file name (root).SRC. The first four records written contain (1) title, (2) date and time of run, (3) data set number, trial number, and total number of isotopes (NTOT), and (4) isotope names. The last record written following each execution of the source model contains NTOT+1 zeroes. The records in between the first four and the last contain time (y) and NTOT source rates (Ci/y). The first four records contain character data. All other records are written in list-directed format. This file is only written when the DVM transport model is implemented.
- IOPT(13) If nonzero, write discharge rates to unit 30. Unit 30 is opened with the name (root).DIS. For this option, a nonzero integer has an additional meaning. If transport of multiple chains is simulated, each chain may be transported with a different time step, and, therefore, the discharge rates for each isotope may be found at different times. When the user inputs a positive integer for this option, NEFTRAN II interpolates the discharge rates found at different times and writes all the isotopes on the the same time scale. If this eption is negative, NEFTRAN II writes the rates for ea ; isotope sequentially by chain, at times corresponding to the time step used for each chain. In either case, the first two records consist of the title, and the execution date and time. The remaining format of (root).DIS depends whether the chains have been put on the same time scale or not. If they are on the same time scale, the remainder of the (root).DIS file consists of the following records: (1) d ta set number, trial number, number of rates, and umber of columns (i.e., total number of isotopes), (2) the name of each isotope, and (3) the simulation time (year) and the integrated discharge (C1) for each isotope. Next, NEFTRAN II writes the time (year) versus discharge rate (Ci/yr) information for each isotope, where the time is printed in the first column and the rate for each isotope is printed in each subsequent column. NEFTRAN II writes rates for each additional trial number and data set in the same format as described above. If the rates are not

put on the same time scale for every chain, NEFTRAN II writes the data set number, the trial number and total number of chains. Next, NEFTRAN II writes the following records to (root).DIS for each chain: (1) the chain number, the number of isotopes in the chain, and the number of times at which discharge rates are provided; (2) the name of each isotope in the chain; and (3) the simulation time and the integrated discharge for each isotope in the chain. The time versus discharge rate for each isotope in the chain is then written by NEFTRAN II. This format is repeated for each subsequent trial number and data set.

- ICPT(14) Not currently used.
- IOPT(15) If nonzero, read from an external file, attached as unit 10 with the n/me (root).SMP, usually containing statistically sampled data. This is done by calling subroutine GETRV to read unit 10 and to perform the user-defined instructions coded there. Subroutine GETRV reads from unit 10 in a list-directed format. The first two variables read are integers JTRIAL and NVAR. JTRIAL is the trial number and NVAR is the number of sampled variables to be read subsequently. Each sampled variable is then read which replaces a input variable that was read in FLOWIN from (root).INP.
- IOPT(16) If monzero, read from an external file, attached as unit 11 and named (root).VEL, sats of fluid velocities that apply for discrete time frames. The data on unit 11 is read in a list-directed format by subroutine FLOWIN as illustrated:

Here N stands for the number of legs in the migration path (see variable NPATH in Section 4.3.2). T_i indicates time (y), L_j denotes the jth leg in the migration path, $V_{i,j}$ is the pore fluid velocity (ft/y), and $S_{i,j}$ is the saturation (dimensionless), for time frame i and leg j. It is assumed that the velocities and saturations associated with time T, apply from time $T_{1\cdot 1}$ to time T_1 , where time T_0 is zero. It is required that $0 < T_1 < T_2 < \ldots < T_m$, where m is the number of time frames specified. The option to use this file is only available when the DVM transport model is being used and, as noted previously, automatically invokes the leg-to-leg transfer algorithm.

IOPT(17) If nonzero, read from an external file, attached as unit 12 and named (root).QSC, sets of flow rates for source calculations that apply for discrete time frames. The data on unit 12 is read in a listdirected format by subroutine FLOWIN in time-flow rate pairs (t_i, Q_i) . Times must be increasing and cover the range of release time to simulation time. Flow rates must be non-negative. This option is only available when the DVM transport model is being implemented.

An example of the template that can be used in the input file for these options is given in Table 4.2.

Table 4.2.

Input Template for External File Options

EXTERNAL FILES, NONZERO -> FILE WRITTEN/READ

O WRITE SOURCE RATES (C1/y) TO (root).SRC (UNIT 25)

0 WRITE DISCHARGE RATES (Ci/y) TO (root).DIS, (UNIT 30)

U NOT CURRENTLY USED

0 READ SAMPLED DATA FOR REPEATED TRIALS FROM (root).SMP (UNIT 10)

O READ TIME-DEPENDENT VELOCITIES FROM (root). VEL (UNIT 11)

0 READ TIME-DEPENDENT SOURCE FLOW FATES FROM (root).QSC (UNIT 12)

Run Options. One dummy title record and six records of single value integer data. As indicated in previous sections, NEFTRAN II may be run by implementing several different models. The run options are flags that indicate which models the user wishes to utilize. The following discussion will list each option and describe the model that is implemented depending on the integer value of the run option. If the user inputs run options that are not consistent (e.g., use mixing-cell source with the analytical solution transport model), a warning message will be printed to the hardcopy output files, but execution will continue. Note that option 22 is only applicable if there is no matrix diffusion and time-dependent velocities are not used. Option Description

- IOPT(18) If zero, use DVM to simulate transport. If nonzero, use the analytic solution.
- IOPT(19) If zero, solve the flow network using the properties input for the network legs and junctions. If nonzero, use the pore velocities input in the Migration Path Array or time-dependent velocities from an external file, (see option 15 above). Note, if velocities are to be used from an external file, this option MUST be nonzero.
- IOPT(20) The leach/solubility option can be 0, 1, or 2 to indicate to the source model to use leach rates only, solubilities only, or both, to determine source rates. This option is only applicable for the DVM transport model.
- IOPT(21) The flow-through/mixing-cell option can be 0, 1, or 2 to indicate to the source model to use the flowthrough source, the mixing-cell source, or to choose one as appropriate to determine source rates. This option is only applicable for the DVM transport model.
- IOPT(22) If zero, leaching occurs at a constant rate. If one, leaching occurs at an exponentially decaying rate. This option is only relevant for the DVM transport model.
- IOPT(23) If nonzero, and other input does not impose its use, the leg-to-leg transfer algorithm will be imposed. This is only applicable when the DVM transport model is being implemented.

An example of the template that can be used in the input file for these options is given in Table 4.3.

Table 4.3.

Input Template for Run Control

RUN CONTROLS

USE DVM (0) OR ANALYTIC SOLN (NONZERO)
SOLVE NETWORK (0) OR INPUT VELOCITIES (NONZERO)
LEACH (0), SOLUBILITIES (1), OR BOTH (2) FOR SOURCE RATES
FLOWTHRU (0), MIXCELL (1), OR CHOOSE (2) FOR SOURCE RATES
CONSTANT (0) OR EXPONENTIAL (1) LEACH RATE MODEL
FORCE (NONZERO) USE OF LEG-TO-LEG TRANSFER ALGORITHM

Debug Print Options. One dummy title record vid 15 records of single value integer data. The debug print options are flags that indicate for NEFTRAN II to print debug information (i.e., information that can be used to isolate problems) to the hardcopy output file, (root).OUT. Consistent with the standard print options, a zero means do not print and a nonzero means print. If the user indicates to print debug information that is not consistent with the run options, as discussed below, a warning message will be printed to the hardcopy output file, and the information will not be printed, but execution will continue.

Option Debug Information Frinted if Option is Nonzero

- IOPT(24) The transport, discharge, and source distribution fractions (applicable for DVM transport only).
- IOPT(25) Diagnostic information for subroutine BAND (applicable for the analytical solution transport model only).
- IOPT(26) Diagnostic information for function GIT (applicable for the analytical solution transport model only).
- IOPT(27) The coefficient matrix and constant vector used to solve for pressure at the leg junctions (relevant only if the flow network is solved).
- IOPT(28) The input read from unit 10 for each call to GETRV (relevant only if option 15 is nonzero).
- IOPT(29) Not currently used.
- IOPT(30) The inventory at release time.
- IOPT(31) Restrictions forced on the code-generated time steps for source and transport (applicable for the DVM transport model only).
- IOPT(32) The leg-junction and the junction-leg connections (applicable only if the flow network is solved).
- IOPT(33) The entire set of time-dependent velocities from the external file, unit 11 (relevant only for the DVM transport model).
- IOPT(34) The atom count summary (applicable only for the DVM transport model).
- IOPT(35) The pressure at each junction and flow rates through each leg (relevant only if the flow network is solved).

- IOPT(36) The leg-to-leg transfer and transport adjustment fractions (relevant only for the DVM transport model and if the leg-to-leg transfer algorithm is being used).
- IOPT(37) The mean time spent as each isotope in each of the subchains as a fraction of the transport time step (only relevant for the DVM transport model).
- IOPT(38) The time-dependent source flow rates (only applicable for the DVM transport model).

An example of the template that can be used in the input file for these options in given in Table 4.4.

Table 4.4.

Input Template for Debug Print Options

DEBUG PRINTS, NONZERO -> PRINT

DVM MULTIPLIERS FOR TRANSPORT, DISCHARGE, AND SOURCE
DIAGNOSTIC INFO FOR SUBROUTINE BAND
DIAGNOSTIC INFO FOR FUNCTION GIT
MATRIX/VECTOR SYSTEM SOLVED FOR FLOW
THE DATA READ FROM UNIT 10
NOT CURRENTLY USED
INVENTORY AT RELEASE TIME
RESTRICTIONS PLACED ON THE TIME STEPS
LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
VELOCITY FIELDS FROM UNIT 11
THE ATOM COUNT SUMMARY
JUNCTION PRESSURES & LEG FLOW RATES
LEG-TO-LEG TRANSFER FRACTIONS
TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN
TIME-DEPENDENT SOURCE FLOW RATES

4.3.2 Problem Size Parameters

One dummy title record and five records of single value integer data, followed by two sets consisting of a dummy array title record and a record of multiple integer data. This set of parameters defines the size of the problem to be simulated by NEFTRAN II (e.g., number of legs, number of junctions, number of isotopes). These parameters must be less than the maximum dimensions allowed (see Section 3.3). The problem size parameters are read in two subsets, integer constants followed by integer arrays. The first subset is read like the options described above, one record per value. The second subset is read in two record-pairs. The first record of each pair is read as a character string, which can be used as an array title for the input template. The second record of the pair contains all the values of the one-dimensional array. The following discussion will list each parameter required and the definition of that parameter. Note that the decay chain inclusion flags are also read here since they help determine the problem size.

Name Definition

First Subset:

NLEG	Number of legs in the network.
NJCT	Number of junctions in the network.
NPATH	Number of legs in the migration path.
NCHNS	Number of decay chains to be input.
NELM	Number of elements input (referenced in Properties Array).

Second Subset (One-dimensional Arrays):

NI An array-title on the first record followed by NCHNS values on the second record, where each value indicates the number of isotopes in each decay chain.

the Element

INCHN An array-title on the first record followed by NCHNS values on the second record. Each value is either 0, 1, or 2, indicating that the decay chain is to be included in source calculations and transported, included in source calculations but not transported, or ignored for both, respectively.

The values for NLEG, NJCT, and NPATH are used to establish the rowdimensions of the Network Leg Properties Array, the Network Junction Properties Array, and the Migration Path Properties Array (all discussed in Section 4.4), respectively. If NJCT is input as zero, it is assumed that the network flow model will not be implemented and the reading of the Network Junction Properties Array is omitted. The Decay Chain Array (Section 4.4.4) has row-dimension equal to the total number of isotopes, found by summing over the NCHNS values of the NI array. The Element Properties Array (Section 4.4.5) has row-dimension equal to the product of NELM and NPATH.

The purposes of the INCHN array are for user-convenience and for reproducibility of source rates. For those applications that require a representation of a complete radionuclide inventory, the Decay Chain Array can be generated to include the entire representation. Then, all or selected decay chains can be transported for a given simulation by flagging appropriate entries in INCHN, which avoids editing of the Decay Chain Array. As discussed in Section 2.3.2, the source mode' of NEFTRAN II apportions isotope solubility according to the element solubility and the internally determined time-dependent mass fraction of the isotope to the element. Since the mass of the element at any time is the sum of masses of the isotopes of that element, source rates that depend on solubilities may differ depending on which decay chains are included. Source rates can be reproduced, therefore, by including the same decay chains in the source calculations, whether they are to be transported or not. One final note about the INCHN array is that an entry of 2 (the decay chain is not used for source or transport) for a chain causes modification of NCHNS and NI. That is, following the reading of the Decay Chain Array, NCHNS is decreased the appropriate amount, the NIarray is compacted, and the information for such a chain is NOT stored. These actions should not affect the user unless multiple data sets are provided, in which case the second data set cannot reference a decay chain that has been discarded (i.e., not included for source or transport) in a previous data set. See Section 4.5 for further discussion of multiple data sets. An example of the template that can be used in the input file for these options is given in Table 4.5.

Table 4.5.

Input Template for Problem Size Parameters

GROUP2 - PROBLEM SIZES

0 NUMBER OF NETWORK LEGS 0 NUMBER OF NETWORK JUNCTIONS 0 NUMBER OF MIGRATION PATH LEGS 0 NUMBER OF DECAY CHAINS INPUT 0 NUMBER OF ELEMENTS INPUT CHAIN1 CHAIN2 CHAIN3 CHAIN4 CHAIN5 CHAIN6 - # MEMBERS PER CHAIN 0 CHN1 CHN2 CHN3 CHN4 CHN5 CHN6 - SRC/TRANS-0, SOURCE-1. NEITHER-2 0

4.3.3 Source and Flow Parameters

One dummy title record and six records of single value floating point data. The physical parameters required on input, defined below, are primarily used to determine source rates. The exception is the last parameter, which is used to convert discharge rates to concentrations for output.

Name Definition

- ACSSFR The fraction of inventory accessed for source calculations.
- VOL The pore volume (ft³) of the accessed source regime, used only if the mixing cell source is implemented.
- QSAREA The product of cross-sectional area normal to flow and porosity (resulting units - ft²). QSAREA is used to convert pore fluid velocity of the first leg in the migration path to fluid flow rate (ft³/y) through the source regime, and is used only if the network is not solved and either solubilities are accounted for or the mixing cell source is used. Note that if timedependent velocities are input, NEFTRAN II uses this parameter to create time-dependent flow rates through the source regime unless time-dependent flow rates through the source are also read from an external file.
- RLCH The leach rate (y⁻¹) used if the source is leachlimited.
- SAL The density (1b/ft³) of fluid in the source regime, used to convert fluid mass to volume for solubility calculations and this value is used only if the fluid flow network is not solved.
- QDAREA The product of cross-sectional area normal to flow and effective porosity (resulting units - ft^2), used to convert pore fluid velocity of the last leg in the migration path to fluid flow rate (ft^3/y) at the discharge point. QDAREA is used only if the flow network is not solved and time-dependent radionuclide concentrations are requested for output (see Section 4.3.1).

If the network is solved (option 18 equals zero), QDAREA and SAL and QSAREA are determined internally. For time-varying flow fields, the flow rate at discharge will vary as the interstitial fluid velocity varies for the last leg in the migration path. Time-dependent fl \ll rates through the repository are accounted for either by using the external time-dependent velocity file (i.e., the velocity of the first leg in the migration path and QSAREA), or the flow rate will be updated periodically with flow rates read from an external file of time-dependent flow rates through the source ((root).QSC), in which case QSAREA is not used. If the analytical transport option is chosen (option 17 is nonzero), variables ACSSFR, RLCH, and (optionally) QDAREA are used. In this case the leach time (τ) for the decaying band source boundary condition is taken to be the reciprocal of the leach rate, RLCH. An example of the template that can be used in the input for these options is given in Table 4.6.

Table 4.6.

Input Template for Source/Flow Parameters

GROUP3 - SOURCE/FLOW PARAMETERS

0.	FRACTION OF INVENTORY ACCESSED
0.	PORE VOLUME CONTAINING SOURCE (ft**3)
0.	PORE-AREA OF SOURCE (ft**2)
0.	LEACH RATE (1/y)
0.	DENSITY OF SOURCE FLUID (1b/ft**3)
0.	PORE-AREA AT DISCHARGE (ft**2)

4.3.4 Time Parameters

One dummy title record, four records of single value floating point data, a record containing a dummy array title, and a record with multiple single value floating point data. All time parameters required by NEFTRAN II are input in years. Like the Problem Size parameters, this set is separated into a subset of constants (in this case floating point constants) and a subset containing an array. The array must be preceded by a characte, record, which can be used as a descriptive title for the input template. The following discussion will list and describe each parameter required in this set.

Name Description

First Subset:

TUB	The i	probl	em	simul	ati	on t	ime.
4. 1. 4.	4.1.1.10	1121111	L N/ 1881	69 J. 531 S. 5 3	L 64 W - B-	PAGE - PC1	A-33250 4

- TRLSE The release time (i.e, the earliest time that contaminated fluid begins to migrate).
- TLCH The time that leaching legins (cannot exceed TRLSE).
- DTSRC The time step for source calculations. Entering zero indicates internal determination by NEFTRAN II.

Second Subset:

DTCHN An array title on the first record followed by NCHNS values on the second record, where each value is the time step for each decay chain input. The array title indicates which time step corresponds to which chain. Entering zero for a chain indicates internal determination of the time step by NEFTRAN II.

For the analytical transport model (option 17 is nonzero), TRLSE and TLCH must be equal and DTSRC and DTCHN are not used. If TRLSE is input less than TLCH, NEFTRAN II sets TRLSE equal to TLCH and writes a warning message to the hardcopy output file ((root).OUT). For time-dependent velocities, it is important that the transport time step be an integer divisor of each time interval, and that internally determined time steps (which can vary from time interval to time interval) have this property. As discussed in Chapter 2, a time interval is defined as the beginning and ending time during which specific steady-state fluid flow velocities are assumed to occur in the migration path legs. Since the user can specify only a single value for all time. NEFTRAN II uses this value as a starting point for each time frame and then decreases it, as necessary, to ensure an integral divisor time step for the time interval. An example of the templace that can be used in the input file for these options is given in Table 4.7.

Table 4.7.

Input Template for Time Parameters

GROUP4 - TIME PARAMETERS

0. TIME TO END OF SIMULATION (y) 0. TIME OF ONSET OF MIGRATION (y) 0. TIME OF ONSET OF LEACHING (y) 0. TIME STEP FOR SOURCE (y) CHN1 CHN2 CHAIN3 CHAIN4 CHAIN5 CHAIN6 - TRANSPORT TIME STEPS BY CHAIN 0. 0. 0. 0. 0. 0.

4.3.5 Increment-Determination Parameters

One dummy title record and 16 records of single value floating point data. Parameters that are used by NEFTRAN II for determining velocity increments, source time steps, transport time steps, and transport space steps are included here. These increment-determination parameters are used only for DVM transport (option 17 is zero) and all parameters have default values in NEFTRAN II. If the first parameter (INCRM) is zero, then all default values will be used and no further input for this data set is required. Otherwise, INCRM must be 16 and a value must be provided for each of the 16 parameters, although a zero indicates the use of the default value for the individual parameter. In the following discussion, after describing each parameter, the default values and recommended sets of values if the default values are not utilized will be presented. Any values different from these recommended should be selected very carefully based on extensive knowledge of the code. Following INCRM and the number of velocity intervals (NVI), seven parameters for finding the source time step, and eight parameters for finding the transport time and space steps are listed. All are read as single-valued parameters, so a descriptive message can follow each value for the input template. The following discussion will list and describe each increment-determination parameter.

Name Description

- INCRM If zero, use default values for all of the remaining parameters in this set and no further input is required for these parameters. Otherwise, a value of 16 must be input, which is the number of parameters (i.e., records) that follow.
- NVI The number of velocity intervals used to distribute velocities for the DVM transport model (defeult 7).
- DTPAR(1) The minimum number of source time steps across the leach time, which is the reciprocal of the leach rate, RLCH (default 5).
- DTPAR(2) The number, which when multiplied by an isotope's half-life, results in a time that must not exceed the isotope's mean migration time, if the isotope is to be considered important for determining the time step for source calculations (default 20).
- DTPAR(3) The multiple of the minimum "important" half-life, providing a lower bound for the source time step (default 0.5).
- DTPAR(4) The multiple of the mean mixing cell residence time to provide a lower bound for the source time step (default 0.2), only used if a mixing cell source is utilized.
- DTPAR(5) The fraction of the minimum mean migration time taken over all important isotopes, which is then compared to mean mixing cell residence time, to decide (if optional) if the mixing cell source model should be used (default 0.1).
- DTPAR(6) The fraction applied to the peak source flow rate to determine a source time step that captures the peak source flow rate (default 0.8). The fraction is multiplied by the peak source rate and this amount is added and subtracted from the peak rate. The times at which these two rates occur determines a time range used to bound the source time step. Only applied for time-varying flow rates through the source.

- DTPAR(7) The minimum number of time steps required to generate source rates (default 20).
- DXDTPA(1) The number, which when multiplied by an isotope's half-life, results in a time that must not exceed the isotope's mean migration time, if the isotope is to be considered "important" for determining the time and space steps for transport (default 10).
- DXDTPA(2) The number of standard deviations in time for important isotopes, providing a lower bound for the transport time step (default 1.5). This parameter is used only for the path-averaged transport to ensure resolution of the breakthrough curve in time.
- DXDTPA(3) The maximum reduction factor that curve resolution restrictions can decrease the time step by (default 0.2). Only applied for path-averaged transport.
- DXDTPA(4) The minimum number of time steps used for transport (default 30). For decalations that utilize timedependent velocities, 30 is divided by the ratio of total simulation time to the length of the current time frame. Either this number or 5, whichever is greater, is used as the minimum number of time steps required for the current time frame.
- DXDTPA(5) The Courant number to be used to initialize the space steps following determination of the time step (default 1.5).
- DXDTPA(6) The minimum Courant number to be used if the first attempt at finding the space steps generates a number of space steps which exceeds dimensions (default 0.75).
- DXDTPA(7) The minimum number of grid blocks for the pathaveraged DVM transport case (default 50).
- DXDTPA(8) The minimum number of grid blocks for each leg for the leg-to-leg transfer implementation (default 7).

In regards to the above description of parameters, the concept of isotope importance is discussed in Section 2.3.2 and 2.4.3, and is based on the mean migration time for each isotope. If a decay chain is included in source but is not transported, all isotopes in that chain are considered to be "not important". Isotopes that do not discharge from their initial inventory during the simulation time have undefined mean migration time and are also considered "not important" in finding space and time steps. Further, if time-dependent velocities are used, all of the above parameters are applied to each time frame and there must be a nominal number of time steps across each time frame (refer to DXDTPA(4)). An example of the template that can be used in the input file for these options is given in Table 4.8.

Input Template For Increment-Determination Parameters

GROUP5 - INCREMENT - DEFERMINATION PARAMETERS

0 USE DEFAULTS (0) OR SUPPLY ALL (16) VALUES

(or)

GROUP5 - INCREMENT - DETERMINATION PARAMETERS

16	USE DEFAULTS (0) OR SUPPLY ALL (16) VALUES
0	# VELOCITY INTERVALS (DEFAULT = 7)
0.	MINIMUM # OF SOURCE TIME STEPS ACROSS LEACH TIME (DEFAULT = 5)
0.	ISOTOPE IMPORTANCE PARAMETER FOR SOURCE DT (DEFAULT = 20)
0.	LOWER BOUND PARAMETER FOR SOURCE DT (DEFAULT = .5)
0.	MIXING CELL PARAMETER FOR SOURCE DT (DEFAULT = .2)
0.	PARAMETER TO DECIDE IF MIXING CELL USED (DEFAULT = .1)
0.	PARAMETER TO ENSURE FEAK SOURCE FLOWRATE CAPTURE (DEFAULT = .8)
0.	MINIMUM # OF TIME STEPS FOR SOURCE (DEFAULT = 20)
0.	ISOTOPE IMPORTANCE PARAMETER FOR TRANSPORT DT (DEFAULT = 10)
0.	CURVE RESOLUTION PARAMETER FOR TRANSPORT DT (DEFADLT = 1.5)
0.	MAX, RED. IN TRANS, DT FOR CURVE RESOLUTION DT (DEFAULT = 0.2)
0.	MINIMUM # OF TIME STEPS FOR TRANSPORT DT (DEFAULT = 30)
0.	THE INITIAL COURANT # TO FIND DX'S (1.0)
0.	MINIMUM COURANT # TO FIND DX'S (0.75)
0.	MINIMUM GRID BLOCKS FOR PATH-AVERAGED TRANSPORT (DEFAULT = 50)
0.	MINIMUM GRID BLOCKS/LEG FOR LEG-TO-LEG TRANSFER (DEFAULT = 7)

The space and time step parameters have default values in NEFTRAN II as indicated above and in sections 2.3.2, 2.4.3, and 2.4.4 These default values are based on the main purpose of NEFTRAN II, which is to be used in a performance assessment methodology (i.e., Monte Carlo statistical study). However, it is recognized that NEFTRAN II has the ability to be applied in a wide range of applications. Consequently, recommended sets of values for the increment-determination parameters that correspond to different levels of accuracy are given in Table 4.9. Level 1, which corresponds to the default values, provides coarse results and is usually adequate for rough analysis and statistical studies. Level 2 is the medium level accuracy and should serve well for generating breakthrough curves and statistical studies. Level 3 is the most accurate and the most time consuming, in general, and should, for the most part, be used only for deterministic runs where detailed breakthrough curves are required. To reiterate, although the user has the option to input any values for these parameters, it is recommended that only the sets of values listed in Table 4.9 be used.

Table 4.9.

Parameter	Level 1 (default)	Level 2	Level 3
DTPAR(1)	5	10	25
DTPAR(2)	20	20	20
DTPAR(3)	0.5	0.3	0.1
DTPAR(4)	0.2	0.1	0.05
DTPAR(5)	0.1	0.1	0.1
DTPAR(6)	0.8	0.8	0.8
DTPAR(7)	20	35	50
DXDTPA(1)	10	10	10
DXDTPA(2)	1.5	0.7	0.35
DXDTPA(3)	0.2	0.1	0.05
DXDTFA(4)	30	50	60
DXDTPA(5)	1.5	1.8	2.0
DXDTPA(6)	0.75	0.95	0.95
DXDTPA(7)	50	100	150
DXDTPA(8)	7	15	25

Recommended Sets of Values for the Increment-Determination Parameters

4.4 Array Input Description

For each array that is input, an array title is included in the input file. The reason for this is to help keep track of data while editing input files using standard text editors. The row c'mension for each array is specified by the Problem Size Parameters (Section 4.3.2). With the possible exception of the Junction Properties Array, all arrays are required input for the initial data set. If multiple data sets are provided, array input is required according to user specification. Both the title and the data must be supplied for any array that is to be read again in a new data set. Refer to Section 4.5 for further discussion on multiple data sets.

Leg properties are required in the first and third arrays. Certain properties are required to solve for flow in the network (e.g., hydraulic conductivity), certain properties are required for transport (e.g., connected porosity), and certain properties are required for both (e.g., leg length). If the pressure equations are not solved, many of the leg properties are not used. However, a value must be provided for each array entry because the input is read in a list-directed format.

4.4.1 Network Lag Properties Array

Three dummy array title records followed by NIEG records containing seven data items. The name of the Network Leg Properties Array is read in three character-formatted records. These are followed by NLEG (Section 4.3.2) records, each containing the seven data items listed and described below. In the following discussion, column numeration is used to indicate a data entry on a record and not a specific column number on that record.

10 - 2 -	a second as	and the second	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	20.00	S	
6011	ATET 1	126.5	ICT 1	DL	101	n -
design of the	100.02.02	 Built-5 	-2-2-2-2	1.00	Sec. 26.1	54 ···

3

7

1 Leg number.

2 Inlet junction number.

Outlet junction number, the sign convention in NEFTRAN II for the flow direction is positive from the inlet to outlet for each leg.

- Leg length (ft).
- 5 Cross-sectional area normal to flow (ft²).
- 6 Hydraulic conductivity (ft/day).
 - Relative brine concentration (dimensionless), zero implies fresh water and one implies saturated brine.

If the network flow equations are not solved, columns 5, 6, and 7 are not used and any nonzero entry in these columns will prompt a warning message to be written to the hardcopy output file, but execution will continue. The inlet and outlet junctions are used in checking flow directions along the migration path and the leg lengths are required to find fluid and species migration times.

An array title that provides a template for input consists of column titles for each of the seven data items required. The column titles indicate data names (e.g., Hydraulic K) and required units (e.g., ft/d). An example of the template that can be used in the input file for this array is given in Table 4.10.

		Ne	twork Leg H	roperties &	rray	
Leg #	inlet jet	Outlet jct	Length (ft)	A'ea (sq-1c)	Hy (raulic K 'ft/d)	Brine Conc.
0	0	0	0.	0.	0.	0.
0	0	0	0.	0.	0.	0.

Input Template for Network Leg Properties Array

4.4.2 Junction Properties Array

Three dummy array title records followed by NJCT records each containing four data items. If the network flow system is not solved, the Junction Properties Array can be omitted. This is detected within NEFTRAN II by the value of NJCT (Section 4.3.2). If NJCT is zero, then the reading of the array-name and array data are bypassed. Otherwise, the array-name and array data are required. If the network is not solved, any nonzero entry in this array will prompt a warning message to be written to the output file, but execution will continue. The name of the Network Junction Properties Array is read in three character-formatted records. These are followed by NJCT records each containing the four data items listed and described below. In the following discussion, column numeration is used to indicate a data entry on a record and not a specific column number on that record.

Column Description

1 Junction number.

2 Elevation of the junction (ft).

- 3 If zero, indicates that pressure is unknown at the junction, else the pressure from column number 4 is used as a known boundary pressure in solving the flow network.
 - 4 Known fluid pressure at the jurction (psi).

An array title that provides a tomplate for input by column consists of column titles for each of the four data items required. The column titles indicate data names (e.g., Pressure) and required units (e.g., psi). An example of the template that can be used in the input file for this array is given in Table 4.11.

	Network Junct	ion Properties /	Az Suly
Jct #	Elevation (ft)	Known Press? No/Yes = 0/1	Pressure (psi)
0	0.	0	0.
0	0.	0	0.
0	0.	0	0.
0	0.	0	0.

Input Template for Network Junction Properties Array

1.4.3 Migration Path Properties Array

Three dummy array title records followed by NPATH records each containing eight data items. The name of the Migration Path Properties Array is read in three character-formatted records. These are followed by NPATH (Section 4.3.2) records each containing the eight data items listed and described below. In the following discussion, column numeration is used to indicate 4 data entry on a record and not a specific column number on that record.

<u>elumn</u>	Description
1	Leg number of the leg in the migration path, based on the leg numbering scheme of the Network Properties Array.
2	Longitudinal dispersivity (ft).
3	Space step (ft). If input as zero, NEFTRAN II will determine the space step internally.
4	Flag indicating whether diffusion from the mobile phase to the immobile phase occurs in this leg (i.e., whether the matrix diffusion model in to be imple- mented for this leg), zero implies no and nonzero implies yes.
5	Interstitial porosity for the mobile phase.
6	Porosity for the immobile phase.
7	Mass-transfer coefficient for diffusion (γ^{-1}) .
8	Interstitial fluid velocity (ft/y).

An array title that provides a template for input by column consists of column titles for each of the eight data items required. The column rities indicate data names (e.g., Velocity) and required units (e.g., ft/y). An example of the template that can be used in the input file for this array is given in Table 4.12.

Table 4.12.

Input Template for Migration Path Properties Array

			Migration	Path Prop	erties Ar	ray	
* `g #	Disp (ft)	DX (ft)	Diffus? N/Y=0/1	Mobile Poros.	Immob Poros	Mass Xfer Coef(1/y)	Velocity (ft/y)
0	0.	0.	0	0.	Ο.	Ó.	Ο.
6	Ο.	2.	0	0.	Ο.	0.	0.
0	0.	0.	0	0.	С.	0.	Ο.

To understand the required input of the Migration Path Array, the different run option combinations that NEFTRAN II is capable of implementing must be understood. In NEFTRAN II, there are ten run option combinations as shown in Table 4.13.

Table 4.13.

Run Option Combinations

sfer?	Force L-to-L Trans	Matrix Diffusion?	Solution Technique	External Verocities?	Network Solved?	
	No	No	DVM	No	Yes	
	Yes	No	DVM	No	Yes	
Yes	Default,	Yes	DVM	No	Yes	
	NA	No	Anl.	No	Yes	
	No	No	DVM	No	No	
	Yes	No	DVM	No	No	
Yes	Difault,	Yes	DVM	No	No	
	NA	No	Anl.	No	No	
Yes	Default,	No	DVM	Yes	No	
Yes	Default,	Yes	DVM	Yes	NG	

The first three columns in Table 4.13 are specified in the run option parameters of Section 4.3.1, which are option numbers 19, 16, and 18, respectively. Column number 4 is decided based on the diffusion flags for all of the legs (column number 4 in the Migration Path Array). The last column is also specified in the run option parameters and is option 23. In conjunction with these different run option combinations, three assumptions contained in NEFTRAN II should be noted. First, the analytical transport model is not equipped to treat matrix diffusion nor time-dependent velocities. Second, if matrix diffusion is implemented for any leg in the migration path or if an external file of velocities is used, then the DVM leg-to-leg transfer algorithm is automatically invoked. Third, implementation of the leg-to-leg algorithm can be forced using option 23. Forcing leg-to-leg transport if matrix diffusion is occurr nr or if time-dependent velocities are being used is not necessary because it is already forced and is listed in Table 4.13 as being "default YES" for these run options. Table 4.14 outlines which columns (and in some cases :ows) are used in the Migration Path Array for the specific run-option combinations listed above.

4.4.4 Decay Chain Array

Three dummy array title records followed by NTOT records each containing eleven data items.

Table 4.14.

Migration Path Array Parameters as a Function of Run Option

I. If the NETWORK IS SOLVED

- Leg numbers are used.
- · Mobile phase porosities are used.
- At least one value (see below) of dispersivity is used.

A. For the ANALYTICAL SOLUTION

 Only one value of dispersivity is used and this is taken from the first row in the array (i.e. the dispersivity for the first leg).

B. For the DVM SOLUTION

- The flags indicating diffusion/no diffusion and the option forcing the leg-to-leg transfer algorithm are used.
 - a. If there is NO DIFFUSION and LEG-TO-LEG TRANSFER has not been forced

Table 4.14. (Continued)

Migration Path Array Parameters as a Function of Run Option

- Transport is calculated over a property-averaged path that only one value of dispersivity and one space step are used, and these are taken from the first row in the array.
- b. If there is NO DIFFUSION and LEG-TO-LEG TRANSFER has been forced
 - Transport is calculated over each leg; therefore, for each leg, a dispersivity and a space step, are used.
- c. If there IS DIFFUSION
 - Transport is calculated over each leg; therefore, for each leg, a dispersivity, a space step, an immobile phase porosity, and a mass transfer coefficient are used.
- II. If the NETWORK IS NOT SOLVED AND AN EXTERNAL FILE IS NOT USED
 - 1. Leg numbers are used.
 - 2. Fluid velocities are used.
 - 3. At least one value (see below) of dispersivity is used.
 - A. For the ANALYTICAL SOLUTION
 - Only one value of dispersivity is used and it is taken from the first row (i.e. the dispersivity for the first leg).
 - B. For the DVM SOLUTION
 - The flags indicating diffusion/no diffusion and the option to force leg-to-leg transfer are used.
 - a. If there is NO DIFFUSION and LEG-TO-LEG TRANSFER has not been forced
 - Transport is calculated over a property averaged path so that only one value of dispersivity and one space step are used, and these are taken from the first row.

Table 4.14. (Concluded)

Migration Path Array Parameters as a Function of Run Option

- b. If there is NO DIFFUSION and LEC-TO-LEG TRANSFER has been forced
 - Transport is calculated over each leg; therefore, for each leg, a dispersivity and a space step, are used.
- c. If there IS DIFFUSION
 - Transport is calculated over each leg; therefore, for each leg, a dispersivity, a space step, a mobile phase porosity, an immobile phase porosity, and a mass transfer coefficient are used.
- III. If the NETWORK IS NOT SOLVED AND AN EXTERNAL FILE IS USED
 - 1. Leg numbers are used.
 - 2. Dispersivities are used.
 - 3. Space steps are used.
 - 4. DVM SOLUTION is required.
 - 5. The flags indicating diffusion/no diffusion and the flag to force leg-to-leg transfer are used.
 - a. If there IS DIFFUSION
 - For each leg; a mobile phase porosity, an immobile phase porosity, and a mass transfer coefficient are used.

The name of the Decay Chain Array is read in three character-formatted records. These are followed by NTOT records each containing the eleven data items listed and described below. Here, as in the code, NTOT represents the total number of isotopes input, found by summing the number of isotopes over decay chains. In the following discussion, column numeration is used to indicate a data entry on a record and not a specific column number on that record.

Column Description

1

Isotope name, in this special case the name MUST be surrounded by single quotes to enable FORTRAN listdirected character input. Atomic mass, used only for solubility calculations and can be set to the atomic number.

- 3 Element index, should match an element index in the Element Properties Array below.
- 4 Local index, refers to index within the decay chain and is used to reference parent(s).
- 5 Local index of parent number 1.
- 6 Local index of parent number 2, cannot be nonzero unless column 5 is nonzero.
- 7 Branching fraction from the decay of parent # 1.
- 8 Branching fraction from the decay of parent # 2.
- 9 The initial inventory (Ci).
- 10 The half-life (y).

2

11 Weighting factor that divides into total integrated discharge for each isotope. This may be useful for performance assessment applications, where the appropriate weighting factor for each isotope may be found based on the EPA Containment Requirements (EPA, 1985), and the resultant weighted integrated discharges would be equivalent to EPA sums.

The element index for all isotopes of a given element should be the same so that solubilities will be treated correctly in the source calculations. The same element retardation is assigned to all isotopes of the element. If weighting factors are input as zero, the default value of 1.0 is used.

An array title that provides a template for input by column consists of column titles for each of the eleven data items required. The column titles indicate data names (e.g., Inventory) and required units (e.g., Ci). An example of the template that can be used in the input file for this array is given in Table 4.15.

4.4.5 Element Properties Array

Three dummy array title records followed by NELM record-sets containing NPATH records. The name of the Element Properties Array is read in three character-formatted records. These are followed by NELM (Section 4.3.2) record-sets, each pertaining to a specified element and each containing NPATH (Section 4.3.2) records. The first record of a set contains element index, solubility, the index of the first leg in the migration path, the mobile phase retardation factor (R_d) for the first leg in the migra-

				De	cay C	hains A	rray			
Name A6	Atom Mass	Ele- ment	Loc ndx	Par #1	Par #2	Frac From1	Frac From2	Inven (Ci)	Hf·Lf (y)	Weigh Fac
'namel'	0	0	0	0	0	0.	0.	0.	0.	0.
'name2'	0	0	0	0	0	0.	0.	0.	0.	Õ.
'name3'	0	0	0	0	0	0.	0.	0.	0.	Ő.

Input Template for Decay Chains Array

tion path. Records 2 through NPATH of a set contain the leg index, the mobile phase R_d , and the immobile phase R_d for legs 2 through NPATH, respectively. Every element index referenced in the Decay Chains Array above should be included in the first column of the Element Properties Array. Each column required in the Element Properties Array is listed below, along with a description of that column. In the following discussion, column numeration is used to indicate a data entry on a record and not a specific column number on that record.

	Column	Description
irst	Record:	
	1	Index of the element.
	2	Solubility (g-element/g-fluid).
	3	Index of the first leg in the migration path.
	4	Mobile $R_{\rm d}$ for the first leg in the migration path.
	5	Immobile $R_{\rm d}$ for the first leg in the migration path.
th Re	cord, I = 2,.	,NPATH:
	1	Index of the Ith leg in the migration path.
	2	Mobile R_d for the $I^{\mbox{\tiny th}}$ leg in the migration path.
	3	Immobile $R_{\rm d}$ for the Ith leg in the migration path

F

Note that the record-set described above must be repeated for each element. Solubilities are not used if only leaching is considered in finding the source rate (option 20, Section 4.3.1). Immobile phase R_d is

not used unless diffusion is being modeled. If nonzero values are input for these parameters for these cases, a warning message is written to the hard copy output file, but execution continues. However, it should be reiterated that, since the array is input in a list-directed format, a blank is not accepted as input for these parameters.

An array title that provides a template for input by column consists of column titles for each of the data items required. The column titles indicate data names (e.g., Solubility) and required units (e.g., g/g). -An example of the template that can be used in the input file for this array is given in Table 4.16.

Table 4.16.

Input Template for Element Properties Array

Elem. Index	Solubility (g/g)	Leg #	Mobil Rd	Immobile Rd
0	0.	0	Ο.	Ο.
		0	0.	0.
		0	0.	0.
0	0.	0	0.	0.
		0	Ο.	0.
		0	0.	0.
0	0.	0	0.	0.
		0	0.	0.
		0	0.	0.

Element Properties Array

Data Required for Multiple Simulations 4.5

For a single run of NEFTRAN II, the run-title, the five sets of parameters, and the five arrays described are required in the input file. Multiple runs of NEFTRAN II can be accomplished using two methods. First, multiple data sets can be included sequentially on the input file. Second, an external file can be read and user-specified replacement statements implemented. In fact, although not routinely done, these two methods can be used together. The two methods are described in the next two subsections.

4.5.1 Multiple Data Sets

One dummy title record and one multiple integer record. For NEFTRAN II, the initial data set is read, and following transport of all chains, the code returns to subroutine FLOWIN to read additional data. If an end-offile is encountered on the input file, the program terminates normally. Otherwise, the code reads the INP array, which contains flags that indicate which data groups are to be re-read. In NEFTRAN II there are 10 data groups that can be flagged. The basic idea is to provide the capability to perform additional calculations without having to re-input those data groups that do not change.

For NEFTRAN II the INP array is read in two records. The first record is a character record that can contain a descriptive title for the second record. The second record contains 10 integers, the first five for the parameter sets and the second five for the arrays. A nonzero entry signifies that the corresponding data-group should be re-read. The following discussion lists each entry in the INP-array and the corresponding data-group that is read again if the entry is nonzero.

- Entry Data-Group to be Re-read if Entry is Nonzero
- 1 Options, Parameter Set 1.
- 2 Problem sizes, Parameter Set 2.
- 3 Source/flow characteristics, Parameter Set 3.
- 4 Time valus, Parameter Set 4.
- 5 Values used to determine space and time increments, Parameter Set 5.
- 6 Network Leg Properties, Array #1.
- 7 Network Junction Properties, Array #2.
- 8 Migration Path Properties, Array #3.
- 9 Decay Chain Properties, Array #4.
- 10 Element Properties, Array #5.

An example of a template that can be used in the input file for this array is given in Table 4.17. The array title consists of column titles for each data group (e.g., set one, set two, array one, array two).

Table 4.17.

Input Template for Multiple Data Set Options

SET1	SET2	SET3	SET4	SET5	ARY1	ARY2	ARY3	ARY4	ARY5	RE-READ	FLAGS	1=>Y
0	0	0	0	0	0	0	0	0	0			

All data-items are subject to error checking during the input of a second or later data set. In addition, if all data groups are not re-read, subroutine STOFPER is called to re-check the entire current data set. This should trap most errors. However, it is recommended that any change in Problem Sizes be accompanied by re-reading all of the affected arrays. In particular, unintended information can be accessed if a decay chain was not included on an earlier data set (see the INCHN Array, Section 4.3.2) and is included in source and/or transport for a later data set.

It should be noted that any external input files are re-wound and re-read for each data set, as long as the option to include such files has not changed. For (root).SMP this means that a second set of repeated trials can be run with different data sets. For (root).VEL and (root).QSC, the re-reading is done mainly for internal code convenience.

4.5.2 Use of Subroutine GETRV

NEFTRAN II allows for the use of an external file to over-write data that was read in the input file. The logic is to first read an input file and, if option 15 is nonzero, to then call subroutine GETRV to (1) read a record from unit 10 ((root).SMP) and (2) implement the user-defined replacement statements that equate NEFTRAN II variable names to the data from unit 10.

In NEFTRAN II, (root).SMP is read until an end-of-file marker is encountered. At that time the program returns to subroutine FLOWIN to read another data set. If one is encountered, unit 10 is re-wound and is ready for a second set of repeated trials. The required structure of unit 10 is discussed in Section 4.3.1.

NEFTRAN II calls subroutine STOPPER following the users replacement statements in subroutine GETRV. In this manner, data checking is available in NEFTRAN II that augments any user-defined data checks defined by the user in GETRV.

4.6 Sample Input File

The purpose of this section is to present a sample input file to summarize the information that has been presented in sections 4.2 - 4.5. Consequently, a sample input file for an arbitrary problem is shown in Table 4.18. Specific sample problems and their corresponding input will be presented in Chapter 5. As shown in Table 4.18, the first record in the input file contains the title for the simulation, "NEFTRAN II SAMPLE INPUT FILE". For the options, all standard prints are requested and two debug prints are requested. From the second subset of options, both source and discharge rate files are to be written. From the run controls, the code is instructed to use the DVM transport model, the pore velocities input in the Migration Path Properties Array, and to consider leaching using a constant leach rate model with a flow-through source, ignoring solubilities and mixing cell effects.

Sample Input File

NEFTRAN II SAMPLE INPUT FILE PARAMETELS, GKOUP1 - OPTIONS, STANDARD PRINT, NONZERO -> PRINT 1 LIST OF ALL PARAMETERS 1 THE NETWORK LEG PROPERTIES ARRAY 1 THE NETWORK JUNCTION PROPERTIES ARRAY 1 THE MIGRATION PATH PROPERTIES ARRAY 1 THE DECAY CHAIN PROPERTIES ARRAY 1 THE ELEMENT PROPERTIES ARRAY 1 FLUID VELOCITIES & SOURCE/DISCH FLOWS 1 SUBCHAINS, PRODUCTION & VELOCITIES 1 SPACE & TIME STEPS AND SOURCE TYPE 1 TIME DEPENDENT OUTPUT, IF +-N, RATES/CONCS EVERY NTH TIME STEP 1 DISCHARGE SUMMARY EXTERNAL FILES, NONZERO -> FILE WRITTEN/READ 1 WRITE SOURCE RATES (Ci/y) TO (root).SRC (UNIT 25) 1 WRITE DISCHARGE RATES (C1/y) TO (root).DIS, (UNIT 30) 0 NOT CURRENTLY USED O READ SAMPLED DATA FOR REPEATED TRIALS FROM (root). SMP (UNIT 10) 0 READ TIME-DEPENDENT VELOCITIES FROM (root). VEL (UNIT 11) O READ TIME-DEPENDENT SOURCE FLOWRATES FROM (root).QSC (UNIT 12) RUN CONTROLS 0 USE DVM (0) OR ANALYTIC SOLN (NONZERO) 1 SOLVE NETWORK (0) OR INPUT VELOCITIES (NONZERO) 0 LEACH (0), SOLUBILITIES (1), OR BOTH (2) FOR SOURCE RATES 0 FLOWTHRU (0), MIXCELL (1), OR CHOOSE (2) FOR SOURCE RATES O CONSTANT (O) OR EXPONENTIAL (1) LEACH RATE MODEL O FORCE (NONZERO) USE OF LEG-TO-LEG TRANSFER ALGORITHM DEBUG PRINTS, NONZERO -> PRINT O DVM MULTIPLIERS FOR TRANSPORT, DISCHARGE, AND SOURCE O DIAGNOSTIC INFO FOR SUBROUTINE BAND O DIAGNOSTIC INFO FOR FUNCTION GIT 0 MATRIX/VECTOR SYSTEM SOLVED FOR FLOW O THE DATA READ FROM UNIT 10 O NOT CURRENTLY USED 1 INVENTORY AT RELEASE TIME 1 RESTRICTIONS PLACED ON THE TIME STEPS 6 LEG/JUNCTION & JUNCTION/LEG CONNECTIONS O VELOCITY FIELDS FROM UNIT 11 O THE ATOM COUNT SUMMARY O JUNCTION PRESSURES & LEG FLOWRATES O LEG-TO-LEG TRANSFER FRACTIONS O TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN O TIME-DEPENDENT SOURCE FLOWPATES

Sample Input File (Continued)

GROUP2 - PROBLEM SIZES 3 NUMBER OF NETWORK LEGS O NUMBER OF NETWORK JUNCTIONS 3 NUMBER OF MIGRATION PATH LEGS 1 NUMBER OF DECAY CHAINS INPUT 3 NUMBER OF ELEMENTS INPUT CHAIN1 CHAIN2 CHAIN3 CHAIN4 CHAIN5 CHAIN6 - # MEMBERS PER CHAIN CHN1 CHN2 CHN3 CHN4 CHN5 CHN6 - SRC/TRANS-0, SOURCE-1, NEITHER-2 0 GROUP3 - SOURCE/FLOW PARAMETERS 1.0 FRACTION OF INVENTORY ACCESSED
 0. PORE VOLUME CONTAINING SOURCE (ft**3)
 0. PORE-AREA OF SOURCE (ft**2) 1.0e-4 LEACH RATE (1/y) O. DENSITY OF SOURCE FLUID (1b/ft**3) 0. PORE-AREA AT DISCHARGE (ft**2) GROUP4 - TIME PARAMETERS 1.0e4 TIME TO END OF SIMULATION (y) 0. TIME OF ONSET OF MIGRATION (y) TIME OF ONSET OF LEACHING (y) 0. 0. TIME STEP FOR SOURCE (y) CHN1 CHN2 CHAIN3 CHAIN4 CHAIN5 CHAIN6 - TRANSPORT TIME STEPS BY CHAIN 0. GROUPS - INCREMENT DETERMINATION PARAMETERS O USE DEFAULTS (O) OR SUPPLY ALL (16) VALUES Network Leg Properties Array Brine Leg Inlet Outlet Length Area Hydraulic # jct jct (ft) (sq-ft) K (ft/d) Conc.
 1
 2
 50.
 0.
 0.

 2
 3
 1000.
 0.
 0.

 3
 4
 2000.
 0.
 0.
 0. 1 1 0. 2 0, 3 Migration Path Properties Array Leg Disp. DX Diffus? Mobile Immob Mass Xfer Velocity # (ft) (ft) N/Y=0/1 Poros. Poros Coef(1/y) (ft/y)

Sample Input File (Cor inued)

					Dec	ay Chai	ns Array	/		
Name A6	Atom Mass	Ele- ment	Loc ndx	Par #1	Par #2	Frac Froml	Frac From2	Inven (Ci)	Hf-Lf (y)	Weigh Fac
10234 TH230	234	1	1	0	0	0.	0.	1000.	2.4E5	0.
RA226	5* 226	3	3	2	õ	1.	0.	3000.	1.6E3	0.
		Eleme	ent Pr	opert	ies A	rray				
Elem Indes	Solub (g/	ility g)	Leg #	, м	lobi1	Rd Im	mobile P	ld		
1	0	. · · ·	1		1.		Ο.			
			2		1.		Ο.			
			3		1.		0.			
4	•		2		1		0.			
			3		1		0			
3	0		1		1.		0.			
			2		1.		0.			
			3		1.		0.			
ETI S	ET2 SET 0 0	3 SET4 0	SET5	ARY1 0	ARY2 0	ARY3 AJ 0	RY4 ARY5 0 0	RE-RE	AD FLAGS	1=>Y
PARAM 1 1 0 7	ETERS, IST OF.	GROUPI ALL PA	- OP RAMET	TIONS ERS PERTI	, STA	NDARD PI	RINT, NO	NZERO -	> PRINT	
0 1	HE NETW	ORK JU	INCTIO	N PRO	PERTI	ES ARRA	Y			
0 T	HE MIGR	ATION	PATH	PROPE	RTIES	ARRAY				
r o	HE DECA	Y CHAI	N PRO	PERTI	ES AR	RAY				
0 7	HE ELEM	ENT PR	OPERT	IES A	RRAY					
OF	LUID VE	LOCITI	ES &	SOURC	E/DIS	CH FLOWS	5			
0 3	UBCHAIN	S, PRC	DUCTI	ON &	VELOC	ITIES				
1 1	TME DED	FUDENT	OUTP	AND S	F + N	LIPE	CONCE F	VERV NT	TTME S	TEP
1 1	1SCHARG	E SUMM	ARY		1	,	CONCS E	V 50 1 1 1 1	a i inis s	1.01
			EX	TERNA	L FIL	ES, NONI	ZERO =>	FILE WR	ITTEN/RE	AD
1 6	RITE SO	URCE R	ATES	(Ci/y) TO	(root).	SRC (UNI	T 25)		
1 6	RITE DI	SCHARG	E RAT	ES (C	1/y)	TO (root	t).DIS,	(UNIT 30))	
ON	OT CURR	ENTLY	USED							1.01
OR	LEAD SAM	PLED D E-DEPE	NDENT	OR RE VELO	PEATE	D TRIALS	S FROM ((root).V	FOOT SN	4Ρ (UNIT Γ 11)	10)

Sample Input File (Concluded)

	RUN CONTROLS
0	USE DVM (0) OR ANALYTIC SOLN (NONZERO)
1	SOLVE NETWORK (0) OR INPUT VELOCITIES (NONZERO)
0	LEACH (0), SOLUBILITIES (1), OR BOTH (2) FOR SOURCE RATES
0	FLOWTHRU (0), MIXCELL (1), OR CHOOSE (2) FOR SOURCE RATES
1	CONSTANT (0) OR EXPONENTIAL (1) LEACH RATE MODEL
0	FORCE (NONZERO) USE OF LEG-TO-LEG TRANSFER ALGORITHM
	DEBUG PRINTS, NONZERO -> PRINT
0	DVM MULTIPLIERS FOR TRANSPORT, DISCHARGE, AND SOURCE
0	DIAGNOSTIC INFO FOR SUBROUTINE BAND
0	DIAGNOSTIC INFO FOR FUNCTION GIT
0	MATRIX/VECTOR SYSTEM SOLVED FOR FLOW
0	THE DATA READ FROM UNIT 10
0	NOT CURRENTLY USED
0	INVENTORY AT RELEASE TIME
0	RESTRICTIONS PLACED ON THE TIME STEPS
0	LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
0	VELOCITY FIELDS FROM UNIT 11
0	THE ATOM COUNT SUMMARY
0	JUNCTION PRESSURES & LEG FLOWRATES
0	LEG-TO-LEG TRANSFER FRACTIONS
0	TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN

O TIME-DEPENDENT SOURCE FLOWRATES

The network for this problem consists of three legs connected end-toend, and the same three legs provide the eligration path. Since the flow network is not solved, it is not necessary to provide junction data; that is, the number of junctions is set to zero. One threemember decay chain is transported and the isotopes are of three distinct elements.

Based on the source run control options, the only required entries from the source and flow parameters are the access fraction and the leach rate. Specifically, the source pore volume is not required (the mixing-cell model is not activated), the pore-area of the source regime is not required (neither the mixing cell nor solubilities are treated), the source fluid density is not required (solubilities are not treated), and the pore-area at discharge is not required (concentration output is not requested). As indicated by the time parameters, simulation is to occur to 10000 years and leaching and fluid flow both start at closure (i.e., zero years). The time steps for source and transport calculations are to be determined by the code.

Only the inlet and outlet junction numbers and the leg lengths are used from the Network Leg Properties Array. Since diffusion from mobile to immobile fluid is not treated for any of the legs in the migration path, NEFTRAN II transports radionuclides over an average, single-porosity path. Thus, the dispersivity and space step are taken from the first row of the digration Path Properties Array and the remaining rows are ignored for these two columns. The space step is input as zero which indicates that NEFTRAN II will determine the space increment internally. Average species velocities are found using the fluid velocities provided in the last column and the retardation factors provided in the Element Properties Array. Mobile phase porosities are not required (the network is not solved and diffusion is not treated), immobile phase porosities are not required (diffusion is not treated).

The Decay Chains Array shows the three-member chain transported with corresponding inventories and half-lives. The normalization (weighting) factors are input as zero so the code defaults them to unity. The element numbering scheme must be consistent with the Element Properties Array. If there were additional isotopes of uranium, for example, either in this chain or subsequent decay chains, all should have element index equal to 1.

The Element Properties Array has NELM (=3) times NPATH (=3) rows. The first row for each element has a different data list than the other rows. Note that each element index in the Decay Chains Array has a corresponding index in the Element Properties Array. Each leg-index in the migration path is repeated for each element. As shown, all elements are not retarded (i.e., $R_d = 1$) for all legs in the migration path. Solubilities are not required (only leaching of waste form is treated) and immobile phase retardations are p^{-r} required (diffusion is not treated).

With the reading of the ninth row of the Element Properties Array, input of the first data set is complete. NEFTRAN II solves for source and transport then returns to subroutine FLOWIN to check for additional data sets. The second data set is initialized by a descriptive header and flags indicating which 'ata groups are to be re-read. For the second data set, some of the options are disabled, but the change of interest is the choice of leach models. For the second data set, the exponential leach rate model is used to determine source rates instead of the constant leach rate model that was used in the first data set.
After reading the options, NENTRAN II performs data checking to help ensure a consistent data set. The code then solves for source and transport using the new options. Following that, it again returns to subroutine FLOWIN to read another data set. At this point, since there is no further input, an end-of-file marker is detected and the program terminates normally.

5.0 VERIFICATION AND SAMPLE PROBLEMS

Three examples of problems simulated with NEFTRAN II are presented in the next three sections. The purpose of these sample problems is to demonstrate the use of different features of the code, as well as to illustrate how NEFTRAN II can be used to simulate different types of problems (e.g., field scale, laboratory scale). The sample problems are also designed to illustrate the process involved in using NEFTRAN II to model real problems since, although NEFTRAN II may appear simple to use, applications of it to real problems require as much thought and analysis as using what might appear to be a more complex code. Each section will include instructions for preparing each input file and each sample problem is also compared with an analytical solution to verify that the computer code has implemented the corresponding mathematical model correctly.

5.1 Sample Problem 1 - DVM and Analytical Transport Model

The first sample problem is designed to demonstrate the use of the flow network model, the use of both the DVM and analytical transport model, the use of multiple data sets, and the ability of DVM to reproduce the analytical solution output. The problem is based on a hypothetical Reference Site, as was presented by Campbell and others (1981b) in the NWFT/DVM user's manual. SWIFT II (Reeves and others, 1986a, 1986b) computer code simulations of the site were used to define the network flow system in NEFTRAN II and to ensure that the network flow model was accurately representing the flow field. The following subsections will present information about the Reference Site, how this information was used to formulate the network flow model in NEFTRAN II, the input required for this problem, and the resultant discharge rate curves for each isotope.

5.1.1 Reference Site

The site is located in a symmetrical upland valley, half of which is shown in Figure 5.1. The crest of the ridge surrounding the valley is at an elevation of 6000 ft. The crest is a surface water and ground water divide. Therefore, ground-water movement in the valley is from water that has fallen in the valley. The valley is drained by a major river, River L, which is at an elevation of 2500 feet opposite the surface structures of the repository.

The geology of the area near the site is shown in cross-section in Figure 5.2. The valley is underlain by crystalline bedrock which crops out over a narrow strip lying at the ridge crest surrounding the valley. The bedrock is assumed impermeable to ground-water flow. The bedrock is overlain by a sequence of sedimentary rocks as shown in Figure 5.2.

SWIFT II computer code simulations of ground-water flow at the Reference Site were conducted. Figure 5.3 shows the direction of ground-water flow schematically. Flow in the upper sand and gravel aquifer is not shown here as it is hydraulically isolated from the middle sandstone by the



ŧ

-





Figure 5.2. Reference Site Geology



Figure 5.3. Ground-Water Flow at Reference Site

upper shale. With the exception of disruptive events, the permeability of the shale and salt is sufficiently low that flow through these layers is generally insignificant. A reduced representation of the Reference Site (the outlined portion in Figure 5.2) was used in the SWIFT II computer code simulations to find pressures. Figure 5.4 shows the resultant pressure head distribution and Figure 5.5 shows the gridding used in the SWIFT II simulations.

Both Figures 5.3 and 5.4 suggest that flow in the middle and lower sandstone aquifers (or some portion of them) can be adequately represented by one-dimensional flow systems. Thus, the network flow model contained in NEFTRAN II can be used to reproduce this flow system.

5.1.2 Network Flow Model

Figure 5.6 shows the NEFTRAN II network superimposed with the darker lines on the Reference Site, and Figure 5.7 shows the NEFTRAN II flow network for this problem with the corresponding leg and junction numbering scheme. Legs 1-4 of the network are placed at the middle shale/middle sandstone interface and legs 5-8 lie at the lower shale/lower sandstone interface. Legs 9, 10, 11, 12, 14 and 15 are used to represent various disruptive features which affect the salt and shale layers near the repository (leg 13) and connect the repository to the overlying aquifer. The left-hand boundary of the network is taken as the midpoint of Column 29 (Figure 5.6) in order to satisfy two restrictions. First, it is of sufficient distance down-dip from the recharge region to ensure that the fluid flow has an insignificant vertical component. Second, it is far enough up dip to ensure that most disruptive features near the repository will not affect the pressure boundary conditions. The resulting emplacement of the NEFTRAN II flow network at the Reference Site is critical to the input of boundary pressures, elevations, and leg lengths.

5.1.3. Data Set #1

The input file for this sample problem is given in Table 5.1. Since Chapter 4 gives detailed instructions for data input, only those input parameters that are specific to this sample problem will be discussed in this section. The user is reminded that, the read statements in NEFTRAN II are list directed; therefore, every parameter and array entry must be assigned a value (i.e., a blank is not permissible).

Options

As indicated in Table 5.1, the user has requested for several different quantities to be written to the hardcopy output file ((root).OUT) by setting the corresponding option to one. Option 8 and 9 are set to zero indicating that the decay/production and velocities of each subchain, and the space step, time increment and source type will not be written to the output file. The user has also indicated to write the discharge rates to an external file, (root).DIS, in the external file options.









Figure 5.5. SWIFT II Gridding for the Reference Site

5-7





.

i.

5-8



1



.

6) Descent 4

Input File for Sample Problem #1

PARA	AN II: SAMPLE PROBLEM #1 FOR USER'S MANUAL (PC VERSION) METERS, GROUP1 - OPTIONS, STANDARD PRINT, NONZERO -> PRINT
1	LIST OF ALL PARAMETERS
1	THE NETWORK LEG PROPERTIES ARRAI
1	THE MIGRATION PATH PROPERTIES ARRAY
1	THE DECAY CHAIN PROPERTIES ARRAY
1	THE ELEMENT PROPERTIES ARRAY
1	FLUID VELOCITIES & SOURCE/DISCH FLOWS
0	SUBCHAINS, PRODUCTION & VELOCITIES
0	SPACE & TIME STEPS AND SOURCE TYPE
1	DISCHARGE SUMMARY
	EXTERNAL FILES, NONZERO -> FILE WRITTEN/READ
0	WRITE SOURCE RATES (Ci/y) TO (root).SRC (UNIT 25)
1	WRITE DISCHARGE RATES (C1/y) TO (root).DIS, (UNIT 50)
0	READ SAMPLED DATA FOR REPEATED TRIALS FROM (root) SMP (UNIT 10)
ŏ	READ TIME-DEPENDENT VELOCITIES FROM (root). VEL (UNIT 11)
0	READ TIME-DEPENDENT SOURCE FLOWRATES FROM (root).QSC (UNIT 12)
	RUN CONTROLS
1	USE DVM (0) OR ANALYTIC SOLN (NONZERO)
0	SOLVE NETWORK (0) OR INPUT VELOCITIES (NONZERO)
0	LEACH (0), SOLUBILITIES (1), C" BOTH (2) FOR SOURCE RATES
0	CONSTANT (0) OR EXPONENTIAL (1) LEACH RATE MODEL
0	FORCE (NONZERO) USE OF LEG-TO-LEG TRANSFER ALGORITHM
	DEBUG PRINTS, NONZERO -> PRINT
0	DVM MULTIPLIERS FOR TRANSPORT, DISCHARGE, AND SOURCE
0	DIAGNOSTIC INFO FOR SUBROUTINE BAND
0	DIAGNOSTIC INFO FOR FUNCTION GIT
0	THE DATA READ FROM UNIT 10
õ	NOT CURRENTLY USED
0	INVENTORY AT RELEASE TIME
0	RESTRICTIONS PLACED ON THE TIME STEPS
1	LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
0	VELOCITY FIELDS FROM UNIT 11
0	THE ATOM COUNT SUMMARY
1	TEC. TO TEC TRANSFER FRACTIONS
0	TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN
0	TIME-DEPENDENT SOURCE FLOURATES
	양감추 방법화 가슴 가슴을 걸 것이 같아. 그는 것이 가지 않는 것이 같아. 이 것이 같아.

1

Input File for Sample Frohlem #1 (Continued)

16 13 5 1 3 CHAI	NUMBER NUMBER NUMBER NUMBER NUMBER N1 CHAI	GROUP2 - OF NETWOR OF NETWOR OF MIGRAT OF DECAY OF ELEMEN N2 CHAIN3	PROBLEM S12 K LEGS K JUNCTIONS ION PATH LEG CHAINS INPUT TS INPUT CHAIN4 CHAI	CES CS CN5 CHAIN6	- ₽ MEMBERS	PER CHAIN
HN1	GHN2 CH	IN3 CHN4 C	HN5 CHN6 - 9	SRC/TRANS-0	, SOURCE-1,	NEITHER-2
1. 0. 0. 1. 0.	0 0e+5	GROUP3 - FRACTION PORE VOLU PORE-AREA LEACH RAT DENSITY O PORE-AREA	SOURCE/FLOW OF INVENTORY ME CONTAININ OF SOURCE E (7 'y) F SOURCE FLU AT DISCHARC	V PARAMETER Y ACCESSED NG SOURCE ((ft**2) UID (1b/ft* GE (ft**2)	s ft**3) **3)	
1. 0. 0. CHN1 0.	Oe5 CHN2 CI	GROUP4 - TIME TO E TIME OF C TIME OF C TIME STEE HAIN3 CHAI	TIME PARAM ND OF SIMUL NSET OF MIG NSET OF LEA FOR SOURCE N4 CHAIN5 C	ETERS ATION (y) RATION (y) CLING (y) (y) HAIN6 - TRA	INSPORT TIME	STEPS BY CHAIN
0	USE 1	GROUP5 - DEFAULTS (Ne	INCREMENT 0) OR SUPPL	DETERMINAT Y ALL (16) roperties /	ION PARAMETE VALUES Array	RS
Leg #	Inlet jct	Outlet jct	Length (ft)	Area (sq-ft)	Hydraulic K (ft/d)	Brine Conc.
1 2 3	1 4 5	4 5 10	1.45e04 8.e03 3.8e04	6.e6 6.e6 6.e6	50. 50. 50.	0. 0. 0.
4	10	3	1.005	6.66	50.	0.

			N 1 41 1 4	0.00	JV .	V.,
3	5	10	3.8e04	6.e6	50.	0.
4	10	3	1.e05	6.66	50.	0.
5	2	9	1.45e04	1.8e6	40.	0
6	9	11	8.e03	1.8e6	40.	0
7	11	12	3.8e04	1.8e6	40.	0.
B	12	13	1.e5	1.8e6	40.	0
9	6	4	6.e02	7.07e2	0.1	0.6
0	8	5	4.965e02	1.0	10.0	1 0
1	9	6	5.e2	1.0	1.678-06	1.0
2	11	8	6.035e2	1.0	1.5e-06	1.0

.

		Input	File	for S	ample	Proble	8m #1	(Continue	ed)		
13	6	7	4	e03	-	5.4eJ	2	10.0		1.0	
14	7	8	4	e03		5.400	2	10.0		1.0	
15	12	10	1	1e03		1.0		1.578-00	6	1.0	
16	13	3	1	1e03		1.298		2.5		0.	
			Netwo	rk Ju	nctio	n Prope	rties	Array			
(575 C)	Jet.	Ele	avatio	on	y	tao - P	ress?	P	ressur	e	
	#	(). Ali	(ft)		N	le/Ye	- 0/1		(psi)		
	1	3.4	60241	e 3		1		4. 1. 1. 4	432.7		
	2	2.1	502/1	е3		1			646.1		
	3	1.1	52589	e3					432.7		
	4	3.4	41481	e3		0			0.		
	5	3.	31131	e3		0			0.		
	6	2.1	81481	0.1		0			0.		
	0	2.1	01/01	e3		0			0		
	0	2.1	21/21	63		0			0.		
	10	2	81067	63		0			0.		
	11	2	21131	e3		Ő			0.		
	12	1	71967	e3		0			0.		
	13	4.	2589e	2		0			0.		
			Mi	gratio	on Pa	th Prop	erties	Array			
Leg	Disp.	DX	Di	ffus?	Mo	bile	Immol	Mass	Xfer	Vel	ocity
#	(ft)	(ft)	N/	Y=0/1	Po	ros.	Poros	s Coet(1/y)	(1	(t/y)
13	500.	0.		0	0	. 3	0.	0.			0.0
14	0.	0.		0	0	.3	0.	0.			0.0
10	0.	0.		0	0	.15	0.	0.			0.0
3	0.	0.		0	0	.3	0.	0.			0.0
4	0.	0.		6	0	. 3	0.	0.			0.0
					Dec	ay Chai	ins Ar	ray	116	1.5	Undek
Name	Atom	Ele-	Loc	Par	Far	Frac	Fra	a inver	i ni	- Lil	Fac
Ab	Mass	ment	Dee	#1	#2	rromi	FIO	mz (01)	(,,	rac
'NP237	7' 237	1	1	0	0	0.		0. 1000), 2.	14E6	2.
'U233'	233	2	2	1	0	1.	R. 6.1	0. 1000). 1,	62E5	1.
'TH229	9' 229	3	3	2	0	1.		0. 1000), 7,	30E3	1.

5-12

1 10 10 1 10 10 10 10 10 10 10 10 10 10	
18018 3.1	
a sector do ter a de	

Element Properties Array Elem, Solubility Leg Mobil Rd Immobile Rd Index (g/g) 4 1 0. 1. 0. 13 1. 14 0. 10 1. 0. 3 6.357e? 0. 4 0 6.357e2 2 13 0. 1. 14 1. 0. 1. 10 0. 6.357e2 3 0. 6.357e2 4 0. 13 3 1. 0. 0. 14 0. 1. 10 1. 0. 3 6.357e2 0. 4 6.357e2 0. SET1 SET2 SET3 SET4 SET: ARY1 ARY2 ARY3 ARY4 ARY5 RE-READ FLAGS 1=>Y 1 0 0 0 0 0 0 0 0 PARAMETERS, GROUP1 - OPTIONS, STANDARD PRINT, NONZERO => PRINT 1 LIST OF ALL PARAMETERS O THE NETWORK LEG PROPERTIES ARRAY 0 THE NETWORK JUNCTION PROPERTIES ARRAY O THE MIGRATION PATH PROPERTIES ARRAY O THE DECAY CHAIN PROPERTIES ARRAY O THE ELEMENT PROPERTIES ARRAY 1 FLUID VELOCITIES & SOURCE/DISCH FLOWS 1 SUBCHAINS, PRODUCTION & VELOCITIES 1 SPACE & TIME STEPS AND SOURCE TYPE 1. TIME DEPENDENT OUTPUT, IF +-N, RATES/CONCS EVERY NTH TIME STEP 1 DISCHARGE SUMMARY EXTERNAL FILES, NONZERO => FILE WRITTEN/READ 0 WRITE SOURCE RATES (C1/y) TO (root).SRC (UNIT 25) 1 WRITE DISCHARGE RATES (C1/y) TO (root).DIS, (UNIT 30) O NOT CURRENTLY USED O READ SAMPLED DATA FOR REPEATED TRIALS FROM (root). SMP (UNIT 10) 0 READ TIME-DEPENDENT VELOCITIES FROM (root). VEL (UNIT 11) 0 READ TIME-DEPENDENT SOURCE FLOWRATES FROM (root).QSC (UNIT 12) RUN CONTROLS O USE DVM (O) OR ANALYTIC SOLN (NONZERO) 0 SOLVE NETWORK (0) 03 INPUT VELOCITIES (NONZERO)

Input File for Sample Problem #1 (Continued)

Input File for Sample Problem #1 (Concluded)

O LEACH (O), SOLUBILITIES (1), OR BOTH (2) FOR SOURCE RATES O FLOWTHRU D), MIXCELL (1), OR CHOOSE (2) FOR SOURCE RATES O CONSTANT (O) OR EXPONENTIAL (1) LEACH RATE MODEL O FORCE (NONZERO) USE OF LEG.TO-LEG TRANSFER ALGORITHM DEBUG PRINTS, NONZERO -> PRINT O DVM MULTIPLIERS FOR TRANSPORT, DISCHARGE, AND SOURCE O DIAGNOSTIC INFO FOR SUBROUTINE BAND O DIAGNOSTIC INFO FOR FUNCTION GIT O MATRIX/VECTOR SYSTEM SOLVED FOR FLOW O THE DATA READ FROM (root). SMP O NOT CURRENTLY USED O INVENTORY AT RELEASE TIME O RESTRICTIONS PLACED ON THE TIME STEPS 0 LEG/JUNCTION & JUNCTION/LEG CONNECTIONS O VELOCITY FIELDS FROM (root). VEL O THE ATOM COUNT SUMMARY **O** JUNCTION PRESSURES & LEG FLOWRATES 0 LEG. TO-LEG TRANSFER FRACTIONS O TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN O TIME-DEPENDENT FLGWRATES THROUGH SOURCE REGIME

For the first data set, option 18 is set to one to implement the analytical solution transport model contained in NEFTRAN II and not the DVM transport model. This is the option that will change in the second data set, which will be discuised in Section 5.1.4. Option 19 is set to zero which invokes the flow wit ark model. As discussed in Section 2.2, when the analytical solution ansport model is being implemented the source wodel contained in NEFTRAN II is not implemented. Consequently, options 20 and 21 are not applicable and are set to zero, as indicated in Table 5.1. The option to invoke leg-to-leg transfer (option 23) is also not applicable when the analytical transport model is being implemented, and is input as zero.

The next set of options shown in Table 5.1 are the debug print options. The user has requested for the leg/junction and junction/leg connections, and the junction pressures and leg flow rates to be printed to the hardcopy output file by setting options 32, and 35, respectively, to one. At this point all the options that are required on input have been defined.

Parameters

The first set of parameters re_{q} uired are the problem size parameters. First, the size of the network needs to be defined, and therefore, the number of network legs, number of network junctions, and number of migration path legs are needed. As shown in Figure 5.7, there are 16 network legs, and 13 network junctions. The migration path is assumed to occur through legs 13, 14, 10, 3 and 4; therefore, 5 legs are in the migration path. This path was chosen arbitrarily for this sample problem. However, in practice, a p/2 licle tracker can be used with the flow simulation results to \leq fine the migration path in the network.

To finish defining the problem size parameters, the number of decay chains, the number of elements, and the decay chain inclusion indexes are required. As indicated in Table 5.1, the user has input one decay chain and three different elements. The chain inclusion index is not applicable when the analytical transport model is being implemented, and, therefore, is input as zero.

The next group of parameters shown in Table 5.1 is the source/flow parameters. Here, the user has indicated that the complete source be accessed (i.e., the access fraction is equal to one) and that the leach rate is $1.0 \times 10^{-5} \text{ y}^{-1}$. In terms of the analytical transport model, the leach 'ime (r) for the concentration boundary condition is taken to be the ecliprocal of the leach rate. The remaining parameters are not required when the analytical (ransport model is being implemented and when output concentrations are not desired (option 10 is positive), and are input as zero.

As shown in Table 5.1, for the time parameters, the user has indicated that the simulation time is one million years, and that release and leaching begin at time zero. The source and transport time steps and the increment-determination parameters are not applicable when the analytical solution is implemented and therefore zero is input for these parameters.

Network Leg Properties Array

Table 5.1 presents the Network Leg Properties Array. The first three columns of this array are easily input based on the resultant NEFTRAN II flow network of the Reference Site shown in Figure 5.7. Column four requires the length of each leg. These lengths can be determined from Figure 5.6. Specifically, from the right edge of the repository to River L midpoint is 138000 ft (length of leg 3 + leg 4). Repository length is 8000 ft (length of leg 13 + leg 14) and is assumed to be level. Leg 14 is assumed to be part of the repository, but not to contain any waste; therefore, leg 13 is designated the source leg for transport and assumed to be 4000 ft. From the left edge of the repository to the aquifer inlets in the flow network is 14500 ft (length of leg 1 and leg 5). Vertical legs must maintain a total length of 1100 ft (length o' leg 9 + leg 11, leg 10 + leg 12, leg 15 and leg 16). Leg 15 is arvitrarily placed 138000 ft (length of leg 7 and leg 8) down dip from legs 10 and 12.

Column five in the Network Leg Properties Array requires the crosssectional area of each leg. For the Reference Site, the aquifer widths are assumed to be that of the repository (6000 ft). Upper and lower aquifer depths (1000 ft and 300 ft, respectively) can be found from Figure 5.6 as well as the width of leg 16 (20000 ft). Based on this data the cross-sectional areas of each leg are given by:

(legs 1 - 4)	$1000 \times 6000 = 6 \times 10^6 \text{ ft}^2$,	(5.1)
(legs 5 - 8)	$300 \times 6000 = 1.8 \times 10^6 \text{ ft}^2$,	(5.2)
(leg 16)	$20000 \times 6000 = 1.2 \times 10^8 \text{ ft}^2$.	(5.3)

The rest of the legs were assigned arbitrary cross-sectional areas since these legs represent disruptive events that may effect the flow system.

The next required input for the Network Leg Properties Array is the hydraulic conductivity of each leg (data column 6). The Reference Site hydraulic properties used in the SWIFT II calculations are shown in Table 5.2. Ar ropriate hydraulic conductivities for legs 1, 2, 3, and 4 are the horiz al conductivity of the middle sandstone. The horizontal conductivity of the lower sandstone is appropriate for legs 5, 6, 7, and 8. The horizontal conductivity of the repository area (leg 13 and leg 14) is assumed to be the five orders of magnitude higher than the conductivity of salt. As the hydraulic conductivity across the salt and shale is essentially vertical, an effective vertical conductivity of salt and shale to legs 9, 10, 11, 12, and 15 is assigned. Similarly, leg 16 represents vortical flow through portions of both the middle and lower sandstone. The differing media can be viewed as providing resistance to flow in series and therefore, one effective conductivity for the differing media can be found. For example, the effective conductivity of leg 16 is given by:

$$R_{16} = R_1 + R_M$$
, (5.4)

where R_{16} is the total resistance to be assigned leg 16, R_L the resistance of lower sandstone, R_H the resistance of middle sandstone,

and:

$$R_{i} = \frac{L_{i}}{K_{i}A_{i}}$$
 (5.5)

where L_i is the length (ft), K_i is the hydraulic conductivity (ft/day), A_i is the cross-sectional area (ft²).

Substituting the appropriate values for each media type into Equation 5.4 and rearranging Equation 5.5, the effective conductivity of leg 16 can be found.

The last column of input data needed for the Network Leg Properties Array is the brine concentration (C) of each leg. The interior legs are assumed to contain saturated brine (C = 1), except for log 9 (assumed C = 0.67), and the aquifer legs are assumed to be fresh water (C = 0).

Table 5.2.

	Horizontal Hydraulic Conductivity (ft/day)	Vertical Hydraulic Conductivity (ft/day)	Porosity
Middle Sandstone	50	1.4	0.3
Lower Shale	10-2	10-3	0.3
Salt	10-5	10-6	0.03
Lower Sandstone	40	7.0	0.3

Reference Site Hydraulic Properties

Network Junction Properties Array

The next input array shown in Table 5.1 is the Network Junction Properties Array. The first column is a listing of each junction in ascending order. The second column requires the elevation of each junction. To find the elevations the SWIFT II simulations are used. SWIFT II flow simulations accounted for the dip angle at the Reference Site. Using the sine of this dip angle and the top center of the SWIFT II y-axis grid blocks as measuring points, the grid block distance vertically (i.e., y =0 to y = 29) is 140000 ft. Since the elevation of the first grid block is known to be 6514 ft, the elevation of the bottom grid block is given by:

The elevation of junction 1 (the upper aquifer inlet) is therefore,

$$4702.41 \text{ ft} + 1100 \text{ ft} = 3602 \text{ ft}.$$
 (5.7)

With this reference point, the leg lengths and dip angle are used to determine the remaining junction elevations.

The next column in the Network Junction Properties Array is the flag that indicates whether the pressure is known at that boundary. For this flow network, pressures at elevation for junctions 1, 2 and 3 are required boundary conditions for the network flow model. Therefore, the flag is set to 1 for junctions 1, 2, and 3 in the third column of the Junction Properties Array. Next, in the Network Junction Properties Array is the actual pressure values for the boundary junctions (in this case, junctions 1, 2 and 3). These pressures are taken from the output of the SWIFT II simulation of the Reference Site. SWIFT II calculates pressures at the top center of each grid block. Junctions 1 and 2 correspond directly to grid blocks in the SWIFT II simulation. Junction 3 is treated somewhat differently. The SWIFT II output indicates that pressures along the elevation of Junction 3 show little change from columna 29 - 65 with a value of approximately 433 psi (see Figure 5.5). However, from columns 66 - 69 pressures increase in order to drive the flow upward to River L. The discharge point in NEFTRAN II is 1100 ft below River L; consequer*ly, there is no need for NEFTRAN II to simulate the pressure increase indicated by SWIFT II. Therefore, the pressure at Junction 3 is assumed to be approximately 433 psi. NEFTRAN II flow calculations are more similar to those of SWIFT II when the input outlet pressure is assumed to be constant and not to increase.

Migration Path Properties Array

The next array shown in Table 5.1, is the Migration Path Properties Array. The first column in this array is the leg number for each leg in the migration path. These leg numbers are in reference to the flow network and, as defined arbitrarily, are legs 13, 14, 10, 3 and 4. The next column in this array requires a dispersivity for each leg. When the analytical solution is being implemented, the only dispersivity that is utilized is the one input for the first leg. As Table 5.1 indicates, a dispersivity of 500 ft is assumed for this problem. The next column in the Migration Path Properties Array is the space step column which is not applicable when the analytical solution is being implemented. Implementation of the matrix diffusion model is also not relevant for the analytical solution transport model and, therefore, data input for the fourth, sixth, and seventh columns of this array are not pertinent and are input as zero.

The column in this array that does requires input data is the mobile phase porosity column. The porosity of legs 3 and 4 are taken from the values for middle sandstone in Table 5.2. The repository, legs 13 and 14, is assigned a porosity one order of magnitude higher than salt, and the leg 10 porosity is assumed to be 0.15. For the last column in this array, zeroes have been input, since the network flow model has been implemented and the user does not need to input pore velocities.

Decay Chain Array

The next array to be presented in Table 5.1 is the Decay Chain Array. The decay chain that is being transported for this sample problem is $^{237}Np \rightarrow ^{233}U \rightarrow ^{27}Th$. For each of these three isotopes, the user has supplied: 1) an isotopic name, 2) the atomic mass of the isotope, 3) an element implex, 4) a local decay chain index, 5) the local index of parent number 1 and 2, 6) the fraction from parent number 1 and 2, 7) the inventory, 8) the half-life and 9) the weighting factor. For this chain, ^{233}U and ^{229}Th each have one parent and each parent decays completely into the daughter (i.e., the fraction from parent number 1 is one). The user has input 1000 Di initial inventory and a weighting factor equal to one for each isotope.

Element Properties Array

The last array to be read in the input file shown in Table 5.1, is the Element Properties Array. The first column is the element index that is equivalent to the element index defined in the Decay Chain Array. The solubilities and the immobile retardation factors required for this array are input as zero since this data is not relevant for the analytical solution implementation. For the mobile phase retardation factors, the only legs that retard any of the isotopes are legs 3 and 4, and for all three isotopes, the retardation factor in these legs is input as 635. Implementation of the analytical solution transport model requires that the retardation factors are equal for all isotopes.

5.1.4 Data Set #2

The next input shown in Table 5.1 is the array (INP) that indicates which input data group will be changed for the next data set. As indicated in Table 5.1, the only data input that will be modified for the next data set is SET1, the options. For the first group of options, the standard print options, the user has indicated that the input arrays will not be written to the output file by setting the corresponding options to zero. The user has requested other information to be printed to the output file by setting the corresponding options to one.

The next set of options that are different from the first data set are the run options. Here, the most significant change between the data sets is accomplished by implementing the DVM transport model instead of the analytical transport model (i.e., setting option 18 to zero instead of one). As discussed in Section 2.3, when the DVM transport model is being implemented, the source model contained in NEFTRAN II is utilized. Consequently, options 20 and 21 are relevant for the second data set. In Table 5.1, option 20 equal to zero indicates that only leaching will be modeled in determining DVM source rates, and option 21 equal to zero indicates that the flow-through source model will be used to distribute the source into the source leg (see Section 2.4.8). Option 23 is input as zero which indicates that the leg-to-leg transfer model will not be implemented for DVM transport. Therefore, DVM transport will be simulated using leg-averaged properties (see Section 2.4). Finally, the debug print options are changed so that no debug information is written to the output file for the second data set. The rest of the required input for this second data set is taken from the data input in the first data set.

In the first data set the user input a zero for some data entries to indicate that these data were not relevant for the analytical transport model. By changing the run option to the DVM transport model, the zeroes that were input in the first data set may have different meanings when used in the second data set. For example, the zeroes that were input for the source time step and transport time step indicate that the code is to determine these time steps internally for the DVM transport model. Other examples can be found in the Migration Path Array (e.g., space step) and the Element Properties Array (e.g., solubility limit).

5.1.5 Results

An example of the output file for this sample problem can be found in Appendix E. As requested by the user on input, the first information written to the output file is the input quantities. The user should note that warnings are written to the output file if data inconsistencies are found but are not fatal. This occurs when data is input but is not used (i.e., if dispersivities would have been input for each leg). The remainder of the output file contains the output information the the user has requested.

Figure 5.8, Figure 5.9 and Figure 5.10 show the resultant discharge rate curves for ²³⁷Np, ²³³U, and ²²⁹Th, respectively. Each figure contains the results obtained utilizing the analytical transport model and the DVM transport model contained in NEFTRAN II. Agreement between the two solutions, for each isotope is quite good and indicates that, for this problem, the DVM transport model reproduces results obtained by an analytical solution. Therefore, the code has implemented the methodiate cal model (the convective-dispersion equation) correctly.

5.2 Sample Problem 2 - Matrix Di fusion

The purpose of this sample problem is to demonstrate the matrix diffusion model capability in NEFTRAN II, and by comparing results to an analytical solution, to verify that the matrix diffusion model contained in NEFTRAN II has implemented the mathematical wodel correctly. This problem also illustrates the process of equating input variables required by the analytical solution to NEFTRAN II input variables.

As discussed in Section 2.4.10, the conceptual model for the matrix diffusion model contained in NEFTRAN II consists of assuming that two phases are present in the transport system, a mobile and an immobile phase. The immobile phase serves as a diffusive sink/source for solutes that are being transported in the mobile phase. This conceptual model could be used to represent transport through connected/dead-end pores, liquid/vapor, and fractures/matrix systems. An analytical solution for this conceptual model is given by van Genuchten and Wierenga (1976) and is used for comparison in this sample problem.

The input required for the analytical solution is taken from van Genuchten and Wierenga (1976) and is listed as follows:

q ~ volumetric flow velocity = 10 cm/day

 $D = dispersion coefficient = 30 cm^2/day$

- ρ = bulk density = 1.30 g/cm³
- L = length of column = 30 cm

f = fraction adsorption sites in mobile region = 0.40







0

Ċ,

Figure 5.9. 233U Discharge Rates for Sample Problem #1



)

.

. 0

Figure 5.10. 229Th Discharge Rates for Sample Problem #1

đ

α · mass transfer coefficient = 0.15 day -1

 $T_1 = dimensionless pulse period = 3.0$

K = distribution coefficient = 0.5 cm3/g

 ϕ = fraction mobile water = 0.65

 θ = water content = 0.40

 $\theta_m = \phi \theta = mobile phase water content = 0.26$

 $\theta_{im} = \theta - \theta_{m} =$ immobile phase water content = 0.14

Before these data can be input into a NEFTRAN II input file, several conversions must be performed to determine the equivalent NEFTRAN II input variables. Each variable given above, and the equivalent NEFTRAN II required input is as follows.

1. water content + porosities

The mobile and immobile water c ... Eiven above are equivalent to the mobile and immobile porosities required by NEFTRAN II.

adsorption data → retardation factors

Utilizing the fraction of adsorption sites in the mobile phase, the bulk density and the distribution coefficient given above, the mobile (R_{η_i}) and immobile phase (R_{im}) retardations required by NEFTRAN II are

$$R_{\rm m} = 1 + \frac{f\rho K}{\theta_{\rm m}} , \qquad (5.8)$$

and

$$R_{im} = 1 + \frac{(1-f)\rho K}{\theta_{im}}$$
, (5.9)

respectively.

volumetric fluid velocity - pore velocity

In NEFTRAN II, assuming a unit cross-sectional area, the volumetric fluid velocity given above is equivalent to the Darcy velocity. Therefore, the pore velocity through the migration path is

$$v_m = \frac{q}{\theta_m}$$
, (5.10)

which must be converted from cm/day to ft/yr for input into NEFTRAN II. By inputting the pore velocity directly into NEFTRAN II, the network flow model is not used and the Network Junctions Froperty Array does not need to be input (set number of junctions equal to zero).

Also, due to the unit cross-sectional area, the fluid volumetric flow rate (Q) through the source, that will be needed to determine source parameters subsequently, is equivalent to q.

4. dispersion coefficient - dispersivity

NEFTRAN II requires input of the dispersivity based on

$$D = \alpha v$$
 . (5.11)

Therefore, using the dispersion coefficient given above, the corresponding dispersivity α can be found from

$$\alpha = \frac{D}{v_{\rm m}} \quad . \tag{5.12}$$

where a in centimeters must be converted to feet for input into NEFTRAN II.

5. mass transfer coefficient - mass exchange coefficient

The mass transfer coefficient given above is equivalent to the mass exchange coefficient used in NEFTRAN II except for units $(day^{-1} must be converted to y^{-1})$.

6. length of column - migration path

Since the network flow model is not being implemented, the flow network is structured only with regard to the migration path. NEFTRAN II requires a minimum of two legs in the migration path, where the first leg acts as a source leg. Consequently, the network is structured to contain two legs which is equivalent to the two legs in the migration path. The only input needed for the Network Properties Array is the length of the first and second leg. The length of the column given above and the length of the sc and leg in the migration path are equivalent except for the units (cen'... ters must be converted to feet). The length of the source leg is assumed to be 10% of the length of the second leg. This is based on making the first leg as small as possible since it is not physically representing any part of the column, but not too small that the DVM model (e.g., time or space step criteria) is effected.

7. no decay → half-life

The van Genuchten and Wierenga (1976) analytical solution does not include radioactive decay. To accomplish this in NEFTRAN 11, the halflife of the input solute should be set relatively high compared to the simulation time, to ensure that decay of the solute does not occur during the simulation.

pulse time → leach rate

To approximate the constant flux boundary condition for the analytical solution (see van Genuchten and Wierenga), the constant leach-limited only, flow-through source model should be implemented in NEFTRAN II, by inputting the appropriate run options. Consequently, one of the required source input parameters is the leach rate. The pulse time given above is in dimensionless pore volume units. This is equivalent to

$$T_1 = \frac{v_m \phi}{L t_1} \tag{5.13}$$

where t_1 is the leach time (in days). Solving for this leach time and taking the reciprocal is the constant leach rate required by NEFTRAN II (days must be converted to years).

9. unit source concentration - initial inventory

Part of the boundary condition for the analytical solution is a constant unit source concentration throughout the pulse period. Requiring a unit source concentration is equivalent in NEFTRAN II to requiring that the source rate S (Ci/yr) be equal to the volumetric flow rate Q (ft^{*}/y) throughout the leach time, with no decay. In other words, S divided by Q must equal 1. In NEFTRAN II the source rs^* for a leach limited only source model is given by

$$S = \frac{C_0}{t_1}$$
 (5.14)

where C_o is the initial inventory. Therefore, substituting S equal to Q, the initial inventory is

$$C_{o} = Q t_{1}$$
 (5.15)

Recall that Q is equivalent to q given above, assuming a unit crosssectional area (convert from cm/day to ft/y).

Applying the above conversions, the resultant NEFTRAN II input file is shown in Table 5.3 and the output file is shown in Appendix E. Because the objective of this problem was to compare the NEFTRAN II results to the analytical solution results, the resultant NEFTRAN II discharge rates for the solute are converted to dimensionless times and relative concentrations. Figure 5.11 shows the breakthrough curve for both the analytical solution and the NEFTRAN II simulation. NEFTRAN II reproduces the analytical solution quite well verifying that, for this data set, the matrix diffusion model in NEFTRAN II is a correct representation of the mathematical governing equations presented by van Genuchten and Wierenga (1976).

Table 5.3.

Input File for Sample Problem #2

NEFTRAN II: SAMPLE PROBLEM #2 FOR PC USER'S MANUAL (PC VERSION) PARAMETERS, GROUP1 - OP". IONS, STANDARD PRINT, NONZERO -> PRINT 1 LIST OF ALL PARAMF'ERS THE NETWORK LEG PAOPERTIES ARRAY 1 THE NETWORK JUNCTION PROPERTIES ARRAY 1 THE MIGRATION P/TH PROPERTIES ARRAY 1 THE DECAY CHAIN PROPERTIES ARRAY 1 THE ELEMENT PROPERTIES ARRAY 1 FLUID VELOCITIES & SOURCE/DISCH FLOWS 1 SUBCHAINS, PRODUCTION & VELOCITIES 1 SPACE & TIME STEPS AND SOURCE TYPE 1 TIME DEPENDENT OUTPUT, IF +-N, RATES/CONCS EVERY NTH TIME STEP 1 DISCHARGE SUMMARY EXTERNAL FILES, NONZERO => FILE WRITTEN/READ C WRITE SOURCE RATES (C1/y) TO (root).SRC (UNIT 25) 1 WRITE DISCHARGE RATES (C1/y) TO (root).DIS, (UNIT 30) 0 NOT CURRENTLY USED 0 READ SAMPLED DATA FOR REPEATED TRIALS FROM (root). SMP (UNIT 10) 0 READ TIME-DEPENDENT VELOCITIES FROM (root).VEL (UNIT 11) O READ TIME-DEPENDENT SOURCE FLOWRATES FROM (root).OSC (UNIT 12) RUN CONTROLS O USE DVM (O) OR ANALYTIC SOLN (NONZERO) 1 SOLVE NETWORK (0) OR INPUT VELOCITIES (NONZERO) O LEACH (O), SOLUBILITIES (1), OR BOTH (2) FOR SOURCE RATES 0 FLOWTHRU (0), MIXCELL (1), OR CHOOSE (2) FOR SOURCE RATES O CONSTANT (O) OR EXPONENTIAL (1) LEACH RATE MODEL O FORCE (NONZERO) USE OF LEG-TO-LEG TRANSFER ALGORITHM DEBUG PRINTS, NONZERO -> PRINT O DVM MULTIPLIERS FOR TRANSPORT, DISCHARGE, AND SOURCE O DIAGNOSTIC INFO FOR SUBROUTINE BAND 0 DIAGNOSTIC INFO FOR FUNCTION GIT 0 MATRIX/VECTOR SYSTEM SOLVED FOR FLOW O THE DATA READ FROM UNIT 10 0 NOT CURRENTLY USED **O** INVENTORY AT RELEASE TIME 1 RESTRICTIONS PLACED ON THE TIME STEPS 0 LEG/JUNCTION & JUNCTION/LEG CONNECTIONS 0 VELOCITY FIELDS FROM UNIT 11 1 THE ATOM COUNT SUMMARY 0 JUNCTION PRESSURES & LEG FLOWRATES 0 LEG-TO-LEG TRANSFER FRACTIONS 1 TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN 0 "IME-DEPENDENT SOURCE FLOWRATES GROUP2 - PROBLEM SIZES

2 NUMBER OF NETWORK LEGS

Table 5.3.

Input File for Sample Problem #2 (Continued)

O NUMBER OF NETWORK JUNCTIONS 2 NUMBER OF MIGRATION PATH LEGS 1 NUMBER OF DECAY CHAINS INPUT 1 NUMBER OF ELEMENTS INPUT CHAIN1 CHAIN2 CHAIN3 CHAIN4 CHAIN5 CHAIN6 - # MEMBERS PER CHAIN CHN1 CHN2 CHN3 CHN4 CHN5 CHN6 - SRC/TRANS-0, SOURCE-1, NEITHER-2 0 CROUP3 - SOURCE/FLOW PARAMETERS 1.0 FRACTION OF INVENTORY ACCESSED 0. PORE VOLUME CONTAINING SOURCE (ft**3) 0. PORE-AREA OF SOURCE (ft**2) 101.458 LEACH RATE (1/y) 0. DENSITY OF SOURCE FLUID (lb/ft**3)
0. PORE-AREA AT DISCHARGE (ft**2) GROUP4 - TIME PARAMETERS 2.628e-2 TIME TO END OF SIMULATION (y) 0. TIME OF ONSET OF MIGRATION (y) 0. TIME OF ONSET OF LEACHING (y) 0, TIME STEP FOR SOURCE (y) CHN1 CHN2 CHAIN3 CHAIN4 CHAIN5 CHAIN6 - TRANSPORT TIME STEPS BY CHAIN 0. GROUP5 - INCREMENT DETERMINATION PARAMETERS 0 USE DEFAULTS (0) OR SUPPLY ALL (16) VALUES Network Leg Properties Array Leg Inlet Outlet Length Area Hydraulic Brine # jet jet (ft) (sq-ft) K (ft/d) Cone. 2 0.098425 0. 0. 3 0.98425 0. 0. 1 1 0. 0. 2 2 3 0; Migration Path Properties Ar ay Disp. DX Diffus? Mobile Immob Mass Xfer Velocity (ft) (ft) N/Y=0/1 Poros. Poros Coef(1/y) (ft/y) Leg Disp. 24 1 2.559e-2 0. 0 0.00 0. 0. 460.889 2 2.559e-2 0. 1 0.26 0.14 301.331 460.889 Decay Chains Array Atom Ele- Loc Par Par Frac Frag Inven Hf-Lf Weigh Mass ment ndx #1 #2 From1 From2 (Ci) (y) Fac Name A6 'SOLUTE' 243 1 1 0 0 0, 0, 1,1811 3000, 1.

Table 5.3.

Input File for Sample Problem #2 (Concluded)

	Eleme	nt Prop	erties Array	
Elem. Index	Solubility (g/g)	Leg #	Mobil Rd	Immobile Rd
1	0.	$\frac{1}{2}$	1.0 2.0	0. 3.786

5.3 Sample Problem 3 - Time-dependent DVM Velocities

The purpose of this sample problem is to demonstrate the ability of NEFTRAN II to transpor radionuclides in a time-varying flow field and to verify that the DVM transport model is implemented correctly for time-dependent velocity conditions.

The analytical solution that is used for the comparison is given by Gelbard (1989). The solution is developed for arbitrary time-dependent fluid-flow velocities and dispersion coefficients. However, the solution is constrained to radionuclides that have identical retardation factors. The boundary and initial condition for the analytical solution are an instantaneous release of radionuclides at time zero from a region $-h \leq x \leq 0$.

Table 5.4 shows the NEFTRAN II input file for this sample problem and Table 5.5 shows the external file that contains the time-varying velocity data. The output file for this sample problem is shown in Appendix E. An attempt was made to use input parameters that may be representative of a HLW repository located in unsaturated, fractured media. This is indicated in the following discussion by including the reference for the data that was used. However, the results should not be considered as indicative of the performance of such a repository.

As shown in Table 5.4, the simulation time for this problem is 80000 years. As indicated in Table 5.5, initially, a constant fluid-flow velocity of 3.0 cm/yr (Travis and others, 1984) is assumed. At 50000 years the fluid-flow velocity is doubled. The basic underlying assumption for this problem is that the flow direction does not change with time, but only the magnitude of the velocity is time-dependent.

The migration path length is taken to be 200 m (Travis and others, 1984), which is equivalent to the length of the second leg. The length of the first leg in the migration path, the source leg, is assumed to be 10% of the length of the second leg. This is done because the analytical solution does not account for transport in the source regime, and therefore, the first leg should be as short as possible without affecting the DVM transport model. The dispersivity for each leg is assumed to be 10% of the length of the leg.



Figure 5.11. Breakthrough Curve for Sample Problem #2

Transport is simulated for the three member chain of 2^{43} Am, 2^{39} Pu and 2^{35} U, with hal[§]-lives of 7593 years, 24400 years and 7.1 x 10⁶ years, respectively, and initial inventories of 6.0 x 10⁵ Ci, 1.3 x 10⁷ Ci, and 7.5 x 10² Ci, respectively. These inventories correspond to the amount of HLW that may be placed in a HLW repository (Sinnock and others, 1984). A retardation factor of 19 is assumed for all the radionuclides.

Table 5.4.

Input File for Sample Problem #3

NEFTRAN II SAMPLE PROBLEM #1 PARAMETERS, GROUP1 - OPTIONS, STANDARD FRINT, NCNZERO => PRINT 1 LIST OF ALL PARAMETEPS 1 THE NETWORK LEG PROPERTIES ARRAY THE NETWORK JUNCTION PROPERTIES ARRAY 1 THE MIGRATION PATH PROPERTIES ARRAY 1 THE DECAY CHAIN PROPERTIES ARRAY 1 THE ELEMENT PROPERTIES ARRAY 1 FLUID VELOCITIES & SOURCE/DISCH FLOWS 1 SUBCHAINS, PRODUCTION & VELOCITIES 1 SPACE & TIME STEPS AND SOURCE TYPE 10 TIME DEPENDENT OUTPUT, IF +-N, RATES/CONCS EVERY NTH TIME STEP 1 DISCHARGE SUMMARY EXTERNAL FILES, NONZERO => FILE WRITTEN/READ 1 WRITE SOURCE RATES (C1/y) TO (root).SRC (UNIT 25) 1 WRITE DISCHARGE RATES (Ci/y) TO (root).DIS, (UNIT 30) 0 NOT CURRENTLY USED 0 READ SAMPLED DATA FOR REPEATED TRIALS FROM (root), SMP (UNIT 10) 1 READ TIME-DEPENDENT VELOCITIES FROM (root).VEL (UNIT 11) 0 READ TIME-DEPENDENT SOURCE FLOWRATES FROM (root).QSC (UNIT 12) RUN CONTROLS 0 USE DVM (0) OR ANALYTIC SOLN (NONZERO) 1 SOLVE NETWORK (0) OR 1NPUT VELOCITIES (NONZERO) 0 LEACH (0), SOLUBILITIES (1), OR BOTH (2) FOR SOURCE RATES

- 0 FLOWTHRU (0), MIXCELL (1), OR CHOOSE (2) FOR SOURCE RATES
- 0 CONSTANT (0) OR EXPONENTIAL (1) LEACH RATE MODEL
- 0 FORCE (NONZERO) USE OF LEG-TO-LEG TRANSFER ALGORITHM

DEBUG PRINTS, NONZERO -> PRINT 0 DVM MULTIPLIERS FOR TRANSPORT, DISCHARGE, AND SOURCE 0 DIAGNOSTIC INFO FOR SUBROUTINE BAND 0 DIAGNOSTIC INFO FOR FUNCTION GIT 0 MATRIX/VECTOR SYSTEM SOLVED FOR FLOW 0 THE DATA READ FROM UNIT 10 0 NOT CURRENTLY USED 0 INVENTORY AT RELEASE TIME

Table 5.4.

laput File for Sample Problem #3 (Continued)

1 RESTRICTIONS .'LACED ON THE TIME STEPS O LEG/JUNCTION & JUNCTION/LEG CONNECTIONS 1 VELOCITY FIELDS FROM UNIT 11 0 THE ATOM COUNT 'UMMARY 0 JUNCTION PRESSURES & LEG FLOWRATES 0 LEG-TO-LEG TRAN . "ER FRACTIONS O TIME SPENT AS LACH ISOTOPE IN A SUBCHAIN 0 TIME-DEPENDENT SOURCE FLOWRATES GROUP2 PROBLEM SIZES 2 NUMBER OF NETWORK LIPS O NUMBER OF NETWORK JUNCTIONS 2 NUMBER OF MIGRATION PATH LEGS 1 NUMBER OF DECAY CHAINS INPUT **3 NUMBER OF ELEMENTS INPUT** CHAIN1 CHAIN2 CHAIN3 CHAIN4 CHAI, 5 CHAIN6 - # MEMBERS PER CHAIN 3 CHN1 CHN2 CHN3 CHN4 CHN5 CHN6 - SRC/TRANS-0, SOURCE-1, 'EITHER-2 0 GROUP3 - SOURCE/FLOW PARAMETERS 1.0 FRACTION OF INVENTORY ACCESSED 0. PORE VOLUME CONTAINING SOURCE (ft**3) 0. PORE-AREA OF SOURCE (ft *2) LEACH RATE (1/y) 1.0e-4 0. DENSITY OF SOURCE FLUID (1b/ft**3) 0. PORE-AREA AT DISCHARGE (ft**2) GROUP4 - TIME PARAMETERS 8.004 TIME TO END OF SIMULATION (y) 0. TIME OF ONSET OF MIGRATION (y) 0. TIME OF ONSET OF LEACHING (y) 1000.0 TIME STEP FOR SOURCE (y) CHN1 CHN2 CHAIN3 CHAIN4 CHAIN5 CHAIN6 - TRANSPORT TIME STEPS BY CHAIN 1000.0 **GROUP5** - INCREMENT DETERMINATION PARAMETERS 0 USE DEFAULTS (0) OR SUPPLY ALL (16) VALUES Network Leg Properties Array Leg Inlet Outlet Length Area Hydraulic Brine jet jet (ft) (sq-ft) & (ft/d) Conc. 1 0. 0.

2

Table 5.4.

Input File for Sample Problem #3 (Concluded)

			Migr	ation	Path	Proper	ties A	rray		
Leg #	Disp. (ft)	DX (ft)	Dii N/N	ffus? 8=0/1	Mo Po	bile ros.	Immob Poros	Mass X: Coef(1)	fer Vel /y) (f	ocity t/y)
$\begin{array}{ccc} 1 & 1 \\ 2 & 1 \end{array}$.0e-5 00	0. 1.5		0 0		0. 0.	0. 0.	0 0	0	.0
				De	cay (Chains A	rray			
Name A6	Atom Mass	Ele- ment	Loc ndx	Par #1	Par #2	Frac Froml	Frac From2	Inven (C1)	Hf-Lf (y)	Weigh Fac
'AM243' 'U239' 'U235'	243 239 235	1 2 3	1 2 3	0 1 2	0 0 0	0. 1. 1.	0. 0. 0.	6.063e5 1.301e7 7.463e2	7.593e3 2.44E4 7.100E8	1.0 1.0 1.0
			EJ	emen	t Pro	perties	Array			
	Eler Inde	B. SO	lubili (g/g)	ty	Leg #	Mobil	Rd	Immobile	Rd	
	1		0.		1	19.		0.		
	2		ο.		1	19.		0.		
	3		0.		1 2	19. 19. 19.		0, 0,		

Table 5.5.

External File of Time-Varying Velocity Data

50000.	1	0.098	1.	
	2	0.098	1.	
80000.	1	0.196	1.	
	2	0.196	1.	

For this sample problem, the source model is assumed to be a constant leach-limited, flow-through source. This model is the best approximation to the instantaneous (in time) source boundary condition of the analytical solution. However, the transport time step is also relevant for this approximation, since the source rate for each isotope is essentially "smeared" over the transport time step. Therefore, the transport time step also needs to be relatively small to try to approximate the source boundary condition. In relation to the DVM transport model, it is difficult to make the time step significantly small to approximate the instantaneous source, since numerical dispersion increases with decreasing time step (see Section 2.4.5).

Figure 5.12 shows the resultant discharge curves for ²⁴³Am, ²³⁸Pu, and ²³⁵U from NEFTRAN II and from the analytical solution. The overall agreement between the analytical solution and NEFTRAN II is reasonable. The slight discrepancy may be due to NEFTRAN II not being able to simulate the instantaneous source term accurately. However, what is significant is that NEFTRAN II is reproducing the general shape of the analytical solution near the time the velocities are changing. This verifies that the DVM transport model for time-dependent fluid velocity conditions has implemented the corresponding mathematical model correctly.




6.0 REFERENCES

- Abramowitz, M. and J. A. Stegun, <u>Handbook of Mathematical Functions</u>. Dever Publication, Inc., New York, 1965.
- Bonano, E. J., P. A. Davis, L. R. Shipers, K. F. Brinster, W. E. Beyeler, C. D. Updegraff, E. R. Shapherd, L. M. Tilton, K. K. Wahi, <u>Demonstration of a Performance Assessment Methodology for High-Level Radioactive Waste Disposal in Basalt Formations</u>, SAND86-2325, NUREC/CR-4759, Sandia National Laboratories, Albuquerque, NM, 1989.
- Campbell, J. E., P. C. Kaestner, B. S. Langkopf, and R. B. Lantz, <u>Risk</u> <u>Methodology for Geologic Disposal of Radioactive Waste: The Network</u> <u>Flow and Transport (NWFT) Model</u>, SAND79-1920, NUREG/CR-1190, Sandia National Laboratories, Albuquerque, NM, 1979.
- Campbell, J. E., D. E. Longsine, and M. Reeves, <u>Risk Methodology for</u> <u>Geologic Disposal of Radioactive Waste: The Distributed Velocity</u> <u>Method of Solving the Convective-Dispersion Equation</u>, SAND80-0717, NUREG/CR-1376, Sandia National Laboratories, Albuquerque, NM, 1980.
- Campbell, J. E. and D. E. Longsine, Distributed Velocity Method of Solving the Convective-Dispersion Equation: 2. Error Analysis and Comparison with Other Methods, <u>Advances in Water Resources</u>, Vol. 4, pp. 109-116, 1981.
- Campbell, J. E., D. E. Longsine, and M. Reeves, Distributed Velocity Method of Solving the Convective-Dispersion Equation: 1. Introduction, Mathematical Theory, and Numerical Implementation, <u>Advances in Water Resources</u>, Vol. 4, pp. 102-108, 1981a.
- Campbell, J. E., D. E. Longsine, and R. M. Cranwell, <u>Risk Methodology</u> <u>for Geologic Disposal of Radioactive Waste: The NWFT/DVM Computer</u> <u>Code User's Manual</u>, SAND81-0886, NUREG/CR-2081, Sandia National Laboratories, Albuquerque, NM, 1981b.
- Cranvell, R. M., J. E. Campbell, J. C. Helton, R. L. Iman, D. E. Longsine, N. R. Ortiz, G. E. Runkle, and M. J. Shortencarrier, <u>Risk Methodology for Geologic Disposal of Radioactive Waste: Final Report</u>, SAND81-2573, NUREG/CR-2452, Sandia National Laboratories, Albuquerque, NM, 1982.
- EPA, <u>40CFR191</u>; Environmental Standards for the Management and Disposal of Spent Nuclear Fuel High-Level and Transuranic Radioactive Waste; Final Rule, Federal Register 50, No. 182, 38066-38089, 1985.
- Gelbard, F., <u>Modeling One-Dimensional Radionuclide Transport Under Time-</u> <u>Varying Fluid Flow Conditions</u>, SAND89-1521, NUREG/CR-5412, Sandia National Laboratories, Albuquerque, NM, 1989.
- Iman, R. L. and M. J. Shortencarrier, <u>A FORTRAN 77 Program and User's</u> <u>Guide for the Generation of Latin Hypercube and Random Samples for</u> <u>Use With Computer Models</u>, SAND83-2365, NUREG/CR-3624, Sandia National Laboratories, Albuquerque, NM, 1984.

- Lester, D. H., G. Jan-en, and H. C. Burkholder, Migration of Radioactive Chains Through an Absorbing Medium, AICHE Symposium Series 152, <u>Adsorption and Ion Exchange</u>, Vol. 71, pp. 202-213, 1975.
- Longsine, D. E., E. J. Bonano, and C. P. Harlan, <u>User's Manual for the</u> <u>NEFTRAN Computer Code</u>, Sandia National Laboratories, NUREG/CR-4766, SAND86-2405, Albuquerque, NM, 1987.
- Reeves, A., D. S. Ward, N. D. Johns, and R. M. Cranwell, <u>Theory and</u> <u>Implementation for SWIFT II. The Sandia Waste-Isolation Flow and</u> <u>Transport Model for Fractured Media. Release 4.84</u>, SAND83-1159, NUREG/CR-3328, Sandia National Laboratories, Albuquerque, NM, 1986a.
- Reeves, M., D. S. Ward, N. D. Johns, and R. M. Cranwell, <u>Data Input Guide</u> for SWIFT II. The Sandia Waste-Isolation Flow and Transport Model for Fractured Media, <u>Release 4.84</u>, SAND83-0242, NUREG/CR-3162, Sandia National Laboratories, Albuquerque, NM, 1986b.
 - Jock, S. Y. T. Lin, and J. P. Brannen. <u>Preliminary Bounds on the Extented Postclosure Performance of the Yucca Mountain Repository Site. Southern Nevada</u>, Sandia National Laboratories, SAND84-1492, Albuquerque, NM, 1984.
- Travis, B. J., S. W. Hodson, H. E. Nuttall, T. L. Cook, and R. S. Rundberg, <u>Preliminary Estimates of Water Flow and Radionuclide</u> <u>Transport in Yucca Mountain</u>, Los Alamos National Laboratory, Los Alamos, NM, LA-UR-84-40, 1984.
- Updegraff, C. D. and C. Lee, <u>DCM3D-A Dual Continuum, 3-D Ground-Water</u> <u>Flow Code for Unsaturated, Fractured, Porous Media</u>, SAND90-7015, NUREG/CR-5536, Albuquerque, NM, 1991.
- van Genutchen, M. Th. and P. J. Wierenga, Mass Transfer Studies in Sorbing Porous Media, I. Analytical Solutions, <u>Soil Science</u> <u>Society of America Journal</u>, Vol. 40, No. 4, pp. 473-480, 1976.

APPENDIX A

Species Velocity Model

Application of the DVM transport model to a radioactive decay chain requires a method for determining the average velocity of atoms that decay to daughter products during a time step, Δt . Consider a chain $I_1 \rightarrow I_2 \rightarrow \ldots \rightarrow I_p$. Without loss of generality, the subscripts can be used to identify the chain (i.e., $1 \rightarrow 2 \rightarrow \ldots \rightarrow p$). The decay rate constants are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_p$.

For a given velocity interval in the calculation of species velocities, the averaged velocity for particles that begin Δt as species 1 and and Δt as species p, v_m (1, ..., p), is given by

$$v_{m}(1, ..., p) = \frac{1}{\Delta t} \sum_{i=1}^{p} \overline{T}_{i} v_{i}$$
 (A.1)

where \overline{T}_i is the average time spent as species i during $\Delta t, \ v_i$ the velocity of the species, and $\sum\limits_{i=1}^p \overline{T}_i = \Delta t$.

In order to find the particle-averaged velocities, \overline{T}_i must be determined for each isotope i.

If species 1 survives decay to time t_1 , decays to species 2 at that time, survives as species 2 to time t_2 , decays to species 3 at that time, etc., then, $0 = t_0 < t_1 < t_2 < \ldots < t_p = \Delta t$ and the probability that species i

survives decay over its allotted time is $e^{-\lambda}i(t_1 - t_{1-1})$

The probability that species i decays to species i+1 over an infinitesimal time interval, dt_i , is given by $\lambda_i = dt_i$.

Thus, the probability that species 1 decays to species p over Δt , a $(1,\ \ldots,\ p,\ \Delta t),$ is the multiple integral of the product of the following independent probabilities,

$$pr(1, \dots, p, \Delta t) = \prod_{i=1}^{p} e^{-\lambda_{i} \left[t_{i} - t_{j+1} \right]} \prod_{i=1}^{p-1} \frac{p-1}{\prod_{i=1}^{n} \lambda_{i}} \prod_{i=1}^{n} dt_{i}, \quad (A.2)$$

with integration limits $(0, t_2)$, $(0, t_3)$, ..., $(0, t_p)$. It can be demonstrated that by integrating the probabilities

$$DP(1, ..., p, \Delta t) = \int_{0}^{t_p} \dots \int_{0}^{t_2} pr(1, ..., p, \Delta t)$$
 (A.3)

the resulting expression is given by the Bateman coefficient

$$DP(1, \ldots, p, \Delta t) = \prod_{i=1}^{p-1} \lambda_i \sum_{\substack{j=1 \\ k \neq j}}^{p-1} \frac{e^{-\lambda_j \Delta t}}{\prod_{\substack{k=1 \\ k \neq j}}}; \quad p \ge 1.$$
(A.4)

To find T_i , the integrand $pr(1, \ldots, p, \Delta t)$ in Equation A.3 is weighted by $t_i - t_{i-1}$, and the resulting integral is divided by DP(1, ..., p, Δt). This is equivalent to the following formulation:

$$\tilde{T}_{1} = \left[\int_{0}^{t} p \dots \int_{0}^{t} t_{1} \operatorname{pr}(1, \dots, p, \Delta t)\right] / DP(1, \dots, p, \Delta t) \quad ,$$
(A.5)

$$\overline{T}_{i} = \left[\int_{0}^{t_{p}} \dots \int_{0}^{t_{2}} t_{i} \operatorname{pr}(1, \dots, p, \Delta t) \right] / DP(1, \dots, p, \Delta t) - \frac{i \cdot 1}{\sum_{j \neq 1} \overline{T}_{j}}$$

for 1 = 2, ..., p-1 and

ł.

$$\overline{T}_{p} = \Delta t - \sum_{i=1}^{p-1} \overline{T}_{i}$$
(A.6)

Before evaluating Equation A.5, one should note that for the purposes of finding the mean time spent as each isotope, the decay chain $I_1 \rightarrow I_2 \rightarrow \ldots \rightarrow I_p$ is equivalent to $1 \rightarrow 2 \rightarrow \ldots \rightarrow p$ where $p = I_p$ and I_1 , I_2, \ldots, I_{p-1} is any permutation of the integers 1, 2, ..., p-1. That is, the particles must spend the same amount of time as each species from 1 to p-1 regardless of the order of the decay sequence. Thus, as shown below, the mean time spent as isotope 1 is found. Subsequently, the mean time spent as isotope i is obtained using the same formula used to find T_1 by interchanging the roles of λ_1 and λ_1 , $i = 2, \ldots, p-1$.

The general formula for the mean time spent as isotope 1 is

$$\bar{T}_{1} = \begin{cases} \frac{p \cdot 1}{\prod \lambda_{1}} & \frac{p \cdot 1}{\prod \lambda_{1}} \\ \frac{i = 1}{p} & \Delta t e^{-\lambda_{1} \Delta t} & \frac{p \cdot 1}{\prod \lambda_{1}} \\ \frac{i = 2}{p} & \Delta t e^{-\lambda_{1} \Delta t} & \frac{i = 2}{p} \\ \prod \lambda_{1} - \lambda_{1} & \prod \lambda_{1} \\ i = 2 & \lambda_{1} & \lambda_{1} \end{cases}$$

(A.7)



where $DP(1, p, \Delta t)$ denotes the production factor that would result from decay directly from species 1 to species p. That is, assume species 2, ..., p-1 are not present in the decay chain so that $I_1 \rightarrow I_p$. The factor DP (1, p, At) is then defined by

$$DP(1,p,\Delta z) = \lambda_1 \frac{e^{-\lambda_1 \Delta t} e^{-\lambda_p \Delta t}}{\lambda_p - \lambda_1}$$
 (A.8)

Similar definitions are used for DP (1, p-1, p, At), DP (1, p-2, p-1, p, At), etc.

In order to reduce numerical errors as much as possible, the exponential terms in Equation A.7, are evaluated using an infinite series. Terms in the infinite series with identical powers of At are collected to create a single series which is then evaluated. The complexity of the resulting series is dependent on the value of p. Currently, NEFTRAN II on'y implements this approach for $p \leq 5$.

Encountering the need to transport a six-member subchain is not anticipated and, in fact, has never been noted. In NEFTRAN II, however, an approximate scheme for subchains of length 6 or greater has been implemented. This scheme is also used if it is judged possible that convergence of the above-mentioned series will be too slow or numerically infeasible. Comparing mean-lives of the species to equal shares of the time step, one of three possibilities must be true:

(a) $\frac{1}{\lambda_{1}} > \frac{\Delta t}{p}$ for all i = 1, ..., p(b) $\frac{1}{\lambda_{1}} \le \frac{\Delta_{-}}{p}$ for all i = 1, ..., p

- (c) for some isotopes k, $\frac{1}{\lambda_{L}} \leq \frac{\Delta t}{p}$

and for the remainder j, $\frac{1}{\lambda_{4}} > \frac{\Delta t}{p}$

In case (a) it can be shown that setting

$$\overline{T}_{1} = \frac{\Delta t}{p}$$
(A.9)

for all i = 1, ..., p is a good approximation. One should note that in this case, average velocities are simply arithmetic averages. In case (b) a good approximation is to set

$$\overline{T}_{i} = \frac{1/\lambda_{i}}{\overline{T}} \Delta t , \qquad (A.10)$$

where

$$\overline{T} = \sum_{i=1}^{p} 1/\lambda_i$$

That is, the time spent as species i during Δt is set to a fraction of Δt defined by the ratio of the measurable of species i to the sum of all mean-lives. Finally, for case (c) those species having the smaller mean-lives are assigned their mean-life,

$$\overline{T}_{k} = \frac{1}{\lambda_{k}}$$
(A.11)

and the time remaining in Δt ,

$$TR = \Delta t - \sum_{k} \frac{1}{\lambda_{k}}$$
(A.12)

is divided evenly among the species with larger mean-lives

$$\overline{T}_{j} = \frac{TR}{p - m}$$
(A.13)

where m is the number of species having the smaller mean-lives.

APPENDIX B

Discharge Model

The discharge model contained in NEFTRAN II consists of multiplying the number of atoms of species r - p, at time t, in grid block N_x by the fraction of species r - p in grid block N_x that discharge as species r. These set of fractions are stored in array F. The determination of array F is the subject of this appendix.

F can be determined in a potentially different manner for each different number of precursors (p). However, with simplifying assumptions concerning velocities and production, it is possible to reduce the cases to p = 0 and $p \ge 1$.

<u>Case 1</u> (p = 0). Here, cnly atoms of species r at t, that discharge as species r during the time increment Δt are of concern. Recall that each grid block has its contents of species r partitioned into N_v equally weighted velocity packets. Packet j is assigned velocity v(j, r), j = 1, ..., N_v. So packet j in grid block N - i + l can contribute to the discharge of species r if

$$v(j, r) * \Delta t \ge (i - 1) * \Delta x . \tag{B.1}$$

The measure of its contribution and the time required to discharge depends on the Courant number (CN),

$$CN(j, r) = v(j, r) \cdot \frac{\Delta t}{\Delta x} \cdot \ge (i - 1)$$
 for contribution (B.2)

A packet may totally or partially traverse the boundary as shown in Figure B.1. The contribution factor of packet j in grid block N_{χ} - $i\,+\,1$ is then,

$$h(j, -) = \begin{cases} CN(j, r) - \left[[CN(j, r)] \right] & \text{for } \left[[CN(j, r)] \right] = i-1 \text{ partial} \\ & \text{contribution} \\ (B.3) \\ 1 & \text{for } \left[[CN(j, r)] \right] = i-1 \text{ total} \\ & \text{contribution} \end{cases}$$

where [[CN]] is the greatest integer less than or equal to CN.





The time to discharge, t(j, r, i), is defined as the time at which the <u>spatial midpoint</u>, m_p , crosses the boundary. That is,

$$t(j, r, i) = \begin{cases} \frac{1}{2} \\ \frac{1}{CN(j, r)} \Delta t & \text{for } \left[[CN(j, r)] \right] > i - 1 \\ \frac{CN(j, r) + i - 1}{2CN(j, r)} \Delta t & \text{for } \left[[CN(j, r)] \right] = i - 1 \end{cases}$$
(B.4)

This time is useful because of the decay of species r. Recalling that packet j is weighted by $(N_\nu)^{-1},$ we write

$$F(r, r, i) = \frac{1}{N_{v}} \sum_{j=1}^{N_{v}} h(j, r) e^{-\lambda_{r} t(j, r, i)} . \qquad (B.5)$$

Note that $NB(r, r) = \left[[CN[N_v, r] + 1] \right]$ (B.6)

<u>Case 2</u> $p \ge 1$. Consider the subcase p = 1 as a model. Suppose an atom of species r - 1 at the beginning of time interval Δt is distance L from the discharge point. We determine the probability that this atom decays to species r and discharges in Δt as the product of probabilities of the following three independent events.

Event 1. The atom is of species type r - 1 after time t_d ,

$$0 < t_d < \Delta t$$
 (B.7)

Event 2. During infinitesimal time dt_d , the atom decays to species type r.

Event 3. The atom remains as species r in the time remaining to discharge.

These events have the probabilities:

.

pr (Event 1) =
$$e^{-\lambda}r-1 d$$

pr (Event 2) = f(r, r - 1) λ r - 1 dt d

pr (Event 3) = $e^{-\lambda} r^{t} R$

where f(r, r - 1) is the decay fraction of species r - 1 to r and t_R is the time remaining to discharge, i.e.,

$$t_{R} = \frac{L + v(r - 1)t_{d}}{v(r)}$$
 (B.8)

Note that v(r) and v(r - 1) are picked from the velocity distributions for species r and r - 1. However, they are chosen from the same velocity subinterval and thus the velocity index j is dropped.

The production fraction of species r by species r - 1 is then found by integrating over possible time (i.e., time range during which atoms of species r - 1 can remain as such and still discharge as species r),

$$P(r, r - 1) = \lambda_{r-1} f(r, r - 1) \int_{T_{1}}^{T_{2}} e^{-\lambda_{r-1}t} de^{-\lambda_{r}} \frac{(L - v(r - 1)t_{d})}{v(r)} dt_{d}$$

$$\lambda_{r}L$$

=
$$\lambda_{r-1} f(r, r-1) e$$
 (B.9)

$$\left[\frac{\frac{1}{v(r-1)}}{\frac{\lambda}{r}} + \frac{\lambda}{v(r-1)}\right]_{e} \begin{bmatrix} \frac{\lambda}{r} + \frac{\lambda}{v(r-1)} \\ \frac{\lambda}{v(r-1)} \end{bmatrix} v(r-1)t_{d} \begin{bmatrix} T_{2} \\ T_{2} \end{bmatrix}$$

The above integration is valid as long as

$$\frac{\lambda_{\mathbf{r}}}{\mathbf{v}(\mathbf{r})} \neq \frac{\lambda_{\mathbf{r}} - 1}{\mathbf{v}(\mathbf{r} - 1)} \quad . \tag{B.10}$$

Otherwise, Equation B.9 is replaced by

$$P(r, r - 1) = \lambda_{r - 1} f(r, r - 1) e^{-\frac{\lambda_{r}L}{v(r)}} \left[T_{2} - T_{1}\right] . \quad (B.11)$$

Here, T_1 and T_2 define the time range during which atoms of species r - 1 can remain as such and still discharge as species r .

There are two conditions that must be met to define T_1 and T_2 . First, one of the velocities must be large enough so that atoms traveling with

that velocity can reach the discharge boundary. Second, the velocity of the daughter isotope, r, must be positive. Relative to the latter, recall that velocities are normally distributed. There are combinations of dispersivity, mean velocity, and time step that will produce negative distributed velocities.

Mathematically, the first criterion above means that max $(v_{r-1}, v_r) \cdot \Delta t \ge L$ and the second means $v_r \ge 0$. With these two criteria met, the following table defines the values T_1 and T_2 :

max (0, t) I	0	0
L/v	min (L/v t)	t

 $v_{r-1} > v_r$ $v_r > v_{r-1} > 0$ $v_r > 0 > v_{r-1}$

where $t_I = (L - v_r \Delta t) / (v_{r-1} - v_r)$.

The basis for T_1 and T_2 is shown for one case $(v_{r-1} > v_r)$. The other cases follow from similar as ang. For the first condition above,

 $v_{r-1} \ \Delta t \ge L$. Thus, the ϵ ms an reach the boundary traveling as the parent (r - 1); however, must not cross the boundary prior to decaying to r. The latest time that decay can occur is therefore given by the travel time to the boundary, $T_2 = L/v_{r-1}$. On the other hand, it is not known from the conditions stated whether atoms can reach the boundary traveling as the daughter. If they can, then decay can occur instantaneously so that $T_1 = 0$. If not, then the atoms must travel for sufficient distance as the parent so that when decay does occur, the distance remaining to the discharge boundary can be covered traveling as the daughter in the time remaining in the time step. This condition can be stated as:

 $v_{r-1} T_1 + v_r (\Delta t - T_1) = L$ (B.12)

Solving for T_1 gives the expression for t_1 above. Note that the condition on the adequacy of the daughter velocity to displace atoms to the discharge point is accounted for by taking the maximum value as shown in the first column.

In order to generalize Equations B.9 and B.11 to cases p > 1, one could consider the set

$$\{t(r - p), \ldots, t(r - 1)\}$$

where t(r - k) denotes the time interval over which species r - k does not decay and travels with velocity v(r - k), $k = 1, \ldots, p$. Then dt(r - k) would be that infinitesimal time for decay from species r - k to species r - (k - 1). In this fashion p - 1 nested integrals must be evaluated. However, finding the 2(p - 1) limits of integration then becomes a formidable task.

As an option we treat the decay of species

$$r \cdot p \rightarrow r \cdot (p \cdot 1) \rightarrow \dots \rightarrow r \cdot 1$$

as a single process over time

$$t_{d} = \sum_{k=1}^{p} t(r + k)$$
 (8.13)

The velocity during time t_d is approximated by the arithmetic average of species' velocities, i.e., define v(rp) by

$$v(rp) = \frac{1}{p} \sum_{k=1}^{p} v(r - k)$$
 (B.14)

This is a reasonable approximation for small t_d (see Appendix A, Species Velocity Model), which is generally the case in this analysis.

Event 1 is then restated as:

Event 1': The atom begins Δt as type r - p and is of type r - 1 at t_d.

Events 2 and 3 remain the same with t_R replaced by

$$t_{R} = \frac{L - v(rp)t}{v(r)}d \qquad (B.15)$$

The probability of event 1' is the Bateman production coefficient over $t_{\rm d},$

$$\sum_{k=2}^{p} f\left(r - k, r - (k - 1)\right) \lambda_{r-k} \sum_{\ell=2}^{p} \left\{ \frac{-\lambda_{r-\ell}t - e^{-\lambda_{r-1}t}}{\prod\limits_{m=1}^{p} \left(\lambda_{r-m} - \lambda_{r-\ell}\right)} \right\}$$
(B.16)

where f(r - k, r - (k - 1)) is the decay fraction of species r - k to species r - (k - 1). The production fraction is then

$$P(\mathbf{r}, \mathbf{r} \cdot \mathbf{p}) = \prod_{k=1}^{p} f\left[\mathbf{r} \cdot \mathbf{k}, \mathbf{r} \cdot (\mathbf{k} \cdot \mathbf{1})\right] \lambda_{\mathbf{r} \cdot \mathbf{k}} \cdot \mathbf{r} \cdot \mathbf{r} \cdot \mathbf{p} \left\{ \sum_{r=1}^{T} \frac{\left[\sum_{k=1}^{p} \frac{-\lambda_{r+1}t}{p} - \frac{-\lambda_{r+1}t}{p}\right]}{\left[\sum_{\ell=2}^{p} \frac{-\lambda_{r-\ell}t}{p} \left(\lambda_{r-m} - \frac{\lambda_{r+1}t}{r-\ell}\right)\right]} e^{-\lambda_{r}\left(\frac{\mathbf{L} - \mathbf{v}(\mathbf{r}\mathbf{p})\mathbf{t}}{\mathbf{v}(\mathbf{r})}\right)} dt_{d} \cdot \mathbf{r} \cdot \mathbf$$

If $\frac{\lambda_r}{v(r)} \neq \frac{\lambda_r \cdot j}{v(rp)}$ for all k = 1, ..., p, then integrating Equation B.17 and rearranging terms yields

$$P(r, r - p) = \prod_{k=1}^{p} f\left(r + k, r + (k + 1)\right) \lambda_{r+k} e^{-\frac{\lambda_{r}}{v(r)}L}$$

$$\sum_{\ell=1}^{p} \left\{ \frac{1}{\prod_{m=1}^{m=1} \left(\lambda_{r-m} + \lambda_{r-\ell}\right)} \left[\frac{1/v(rp)}{\lambda_{r}} + \frac{\lambda_{r-\ell}}{v(rp)} e^{\left(\frac{\lambda_{r}}{v(r)} + \frac{\lambda_{r-\ell}}{v(rp)}\right)v(rp)t} e^{\left(\frac{\lambda_{r}}{T_{1}}\right)} \right] \right\}.$$

$$(B.18)$$

If for p = 1 we define $\prod_{m=1}^{p} \left(\lambda_{r-m} - \lambda_{r-\ell} \right) = 1$, then Equation B.18 contains Equation B.9.

If for some $\ell = \ell'$, $\lambda_r/v(r) = \lambda_{r-\ell'}/v(rp)'$ then the sum $\sum_{\ell=1}^{p} l = 1$ $\sum_{\ell=1}^{p} \ell = 1$ $\ell \neq \ell'$

B - 7

$$\prod_{k=1}^{p} f\left(r - k, r - (k - 1)\right) \lambda_{r-k} = \frac{\lambda_{r}}{v(r)} L \frac{T_{2} - T_{1}}{\prod_{m=1}^{p} \left(\lambda_{r-m} - \frac{1}{c-\ell'}\right)}$$
(B.19)
$$\prod_{m=1}^{m-1} \frac{m}{m \ell'}$$

is added.

The determination of T_1 and T_2 proceeds as above with $\nu(r$ - 1) replaced by $\nu(rp)\,.$

Since v(r) = v(j, r) for some velocity interval j = 1, ..., NV, v(rp) and thus P(r, r - p) depend on j. For a given g id block index i define the distance

$$L = \left(i - \frac{1}{2}\right) \Delta x \qquad (B.20)$$

and factor

$$P'(j,r,r-p) = \begin{cases} P(j,r,r-p) & (evaluated at L) & if P(j,r,r-p) > 0 \\ 0 & , & otherwise \end{cases}$$

Finally, array F is defined by

$$F(r, r - p, i) = \frac{1}{N_v} \sum_{j=1}^{N_v} P'(j, r, r - p)$$
(B.21)

It may happen that v(j, r) and v(j, rp) are such that

$$0 < v(j, r) \Delta t, v(j, rp) \Delta t < \Delta x/2$$
 (B.22)

for all j = 1, ..., N_v . In this case, some of species r in grid block N_x should discharge during Δt . However, because we take L as the distance from the grid block midpoint to the discharge location (i.e., for block N_x , L = $\Delta x/2$), the discharge model presented above would produce no discharge of species r. In this special case, L is decreased to L' such that

$$v(j, r) \Delta t > L'$$
 or $v(j, rp) \Delta t > L'$

for some j values. Then for grid block N_x (i.e., i = 1),

$$F(r, r - p, i) = \frac{L'}{L} \frac{1}{N_v} \sum_{j=1}^{v} P'(j, r, r - p)$$
 (evaluated at L') (B.23)

N

Further, note that NB(r, r - p) can be defined by the maximum value of i that yields $P'(j, r, r - p) \neq 0$ for any j.

Recalling that Equation B.18 contains Equation B.9, Equations B.18 and B.23 completely define array F.

APPENDIX C

Distribution of Source Into Migration Path Using Mixing-Cell Model

The mixing-cell source model provides constant, average source rates for radionuclides during each time step, Δt . As radionuclides exit the cell, they enter a ground-water travel path to the accessible environment. Radionuclides traveling along this path are subject to convection, dispersion, retardation, and decay. If an atom exits the mixing cell at time t_c , $t \leq t_c \leq t + \Delta t$, its location at $t + \Delta t$ is subject to all of these processes. The model described below keeps track of the movement of source particles and thus is able to spatially distribute the mass of a species over each Δt .

A source factor array S_p is generated during the initial execution phase of NEFTRAN II. It theoretically has three indices,

$$S_{p} = S_{p}(1, \ell, k) \tag{C.1}$$

where the mass of species i in grid block k will be incremented by fraction $S_F(i,\ell,k)$ applied to the average source of the parent species ℓ . Letting $\rho(i,k,t)$ be the atoms of species i in grid block k at time t, this at time t + Δt is given by

$$\rho(i,k,t + \Delta t) = \rho(i,k,t) + \sum_{i=0}^{P_i} S_F(i,i-j,k)\widehat{S}(i-j)$$
 (C.2)

where P_i is the number of parents necessary to describe production of species i over Δt and S(i-j) is the average source of parent i-j over Δt . S_F is determined separately for the three cases j=0, j=1, j>1.

The DVM technique for radionuclide transport treats convection and retardation by assigning mean velocities to each species, and dispersion is modeled by distribution species velocities about the mean velocity. The species velocities are assumed to have equal probability and there are in general N_o such values (see Section 2.4).

 v_b^i denotes the velocity of species i in velocity bin b, b = 1, ..., N_v. Each atom of species i is therefore assigned a velocity v_i , for a given b after the atom exits the mixing cell at time t_c.

First, the case j=0 will be examined. The fraction $S_F(i,i,k)$ for grid block k is found by integrating the product of the following three probability functions over the total time necessary for particles to be in grid block k at the end of Δt .

1. The probability that an atom exits the cell during the infinitesimal time dt about t is

since S is constant over At.

2. The probability that an atom of species 1 survives decay from $t_{\rm c}$ to the end of Δt is

 $e^{-\lambda_{i}(\Delta t - t_{c})}$ (C.4)

3. The probability that an atom of species 1 is assigned to velocity bin b is $1/N_{\rm v}.$

Therefore, the probability that an atom of species 1 in velocity bin b exits the cell during Δt and occupies grid block k at species 1 at the end of Δt is

$$pr(i,b,k) = \frac{1}{N_v \Delta t} \int_{T_1}^{T_2} e^{-\lambda_i (Wt - t_c)} dt_c$$
, (C.5)

where T_1 and T_2 define the time interval over which an atom can cross the cell boundary and end up in grid block k during Δt .

Integration of Equation C.5 from T₁ to T₂ yields

$$pr(i,b,k) = \frac{1}{\lambda_i \Delta t N_v} \begin{pmatrix} e^{-\lambda_i (\Delta t - T_2)} & -\lambda_i (\Delta t - T_1) \\ e^{-\lambda_i (\Delta t - T_1)} \end{pmatrix}. \quad (C.6)$$

It remains to find T_1 and T_2 . First, one should note the grid block numbering system of Figure C.1. Following the usual treatment of dispersion governed by Fick's first law of diffusion, it is sometimes necessary to allow particles to be dispersed upstream in the migration path. Therefore, some material may appear to move in a negative direction, which is solely the effect of dispersion. This does not imply that particles reenter the cell. Nevertheless, grid block k represents the spatial increment from k Δx to $(k + 1)\Delta x$. Further, only particles assigned positive velocities can end up in positive blocks, and those with negative velocities in negative blocks.



Figure C.1. The Grid Block Numbering Convention

Times T_1 and T_2 are found by noting that the distance traveled by an atom of species i in velocity bin 5 must be bounded by $k\Delta x$ and $(k + 1)\Delta x$ to reside in block k at the end of Δt . That is,

$$k\Delta x \le v_i^b(\Delta t - t_c) \le (k+1)\Delta x$$
 (C.7)

а.

or

$$k\Delta x - v_i^b\Delta t \leq -v_i^b tc \leq (k+1)\Delta x - v_i^b\Delta t$$

If $v_{i}^{b} > 0$, $\Delta t - \frac{(k+1)\Delta x}{v_{i}^{b}} \le t_{c} \le \Delta t - \frac{k\Delta x}{v_{i}^{b}}$ (C.8)

and if $v_b^i < 0$

$$\Delta t - \frac{k\Delta x}{v_b^i} \leq t_c \leq \Delta t - \frac{(k+1)\Delta x}{v_b^i} , \qquad (C.9)$$

The bounds on t_c given by Equations C.8 and C.9 are Δt less the travel times from the cell to the edges of grid block k. These bounds are labeled

$$t_1 = \Delta t - \frac{(k+1)\Delta t}{v_1^b}$$
 and $t_2 = \Delta t - \frac{k\Delta x}{v_1^b}$

respectively. From the grid block numbering convention $t_1\leq \Delta t$ and $t_2\leq \Delta t$. The conditions $v_1^b>0$ and $v_1^b<0$ car be combined by defining T_1 and T_2 as follows

$$T_1 = \max(\min(t_1, t_2), 0)$$
 (C.10)

$$T_{2} = \max(t_{1}, t_{2})$$
 (C.11)

If $t_2 \leq 0$ there is no contribution from velocity bin b to grid block k. In that case, set

$$pr(i,b,k) = 0$$
 . (C.12)

Finally define

$$S_{F}(i,i,k) = \sum_{b=1}^{N_{V}} pr(i,b,k)$$
 (C.13)

for each block k. Since j=0, that is species i has no parents, it follows from Equation C.2 that the second index for S_F must be i.

Next, the case j=l (i.e., a two-member chain) is examined. For convenience, in the notation species i is assumed to decay to species 2. The change in mass of species 2 in each grid block k due to the radio-active decay of species i must be determined. In finding S, it is assumed that decay and production can only occur after an atom exits the cell. Therefore, if t_o is the time at which decay occurs, then $t_d \ge t_c$.

The probability that an atom leaving the cell as species 1 resides in block k as species 2 at the end of Δt is the integral of the product of the following five probabilities.

1. The probability that an atom of species 1 exits the cell during dt_ about t_ is

dt /At

2. The probability that an atom of species 1 survives decay from $t_{\rm c}$ to $t_{\rm d}$ is

$$\lambda_1(t_d - t_c)$$

3. The probability that an atom of species 1 decays to species 2 during dt_d about t_d is

where $h_{1,2}$ is the branching fraction from species 1 to species 2.

4. The probability that an atom of species 2 survives decay from ${\rm t}_{\rm d}$ to Δt is

 $e^{-\lambda_2(\Delta t - t_d)}$

5. The probability that an atom is assigned to velocity bin b is $1/N_v$. It is assumed that, if an atom is assigned velocity v_i^b , then it doesn't change bins after decay. That is, as species 2, it travels with velocity v_i^b .

Therefore, the probability that a source particle of species 1 ends up in block k as species 2 is

$$pr(2,1,k,b) = \frac{h_{1,2}\lambda_1 e^{-\lambda_2 \Delta t}}{\Delta t N_v} \int_{T_{d_1}}^{T_{d_2}} \int_{T_{c_1}}^{T_{c_2}} e^{\lambda_1 t_c}$$
(C.14)

where T_{c1}, T_{c2}, T_{d1}, T_{d2}, define the time ranges to exit the cell and decay so that a particle may occupy block k at the end of Δt .

 $\cdot e^{-(\lambda_1 - \lambda_2)} t_d dt_c dt_d$

In order to solve Equation C.14, the limits of integration must be determined. Disregarding the dependence on K, the integration limits would be

$$T_{c_1} = 0 \qquad T_{d_1} = 0$$
$$T_{c_2} = t_d \qquad T_{d_2} = \Delta t$$

Applying these limits to Equation C.14 then gives the total amount of species 2 produced from decay of species 1. The integration limits are graphically illustrated in Figure C.2.

As well be shown, for an atom to end up in grid block k, the area of integration must also be bounded by a pair of parallel lines. The manner in which these lines intersect the shaded triangle in Figure C.2 results in 36 different sets of limits for T_{d_1} , T_{d_2} , T_{c_1} , and T_{c_2} .



Figure C.2. Shaded Area Represents the Region of Integration for Total Source of Species 2 from Species 1

First, the parallel lines must be determined. The total distance traveled by an atom in velocity bin b is

$$v_1^b (t_d - t_c) + v_2^b (\Delta t - t_d)$$

The superscript b will be dropped for convenience. In order to occupy block k, the following condition must be satisfied

$$k\Delta x \le v_1(t_d - t_c) + v_2(\Delta t - t_d) \le (k + 1)\Delta x$$
 . (C.15)

Solving for t_d directly is possible only when $v_1 \neq v_2.$ If $v_1 > v_2.$ Equation C.15 becomes

$$\frac{k\Delta x + v_2 \Delta t}{v_1 + v_2} + \left(\frac{v_1}{v_1 + v_2}\right) t_c \le t_d \le \left(\frac{v_1}{v_1 + v_2}\right) t_c + \frac{(k+1)\Delta x + v_2 \Delta t}{v_1 + v_2} \quad . \quad (C.16)$$

If $v_1 < v_2$, Equation C.15 becomes

$$\frac{(k+1)\Delta x + v_2\Delta t}{v_1 + v_2} - \left(\frac{v_1}{v_1 + v_2}\right) t_c \le t_d \le \left(\frac{v_1}{v_1 + v_2}\right) t_c + \frac{k\Delta x + v_2\Delta t}{v_1 - v_2}$$
(C.17)

If $v_1 = v_2$, Equation C.15 becomes

$$T_1 \le t_c \le T_2 \tag{C.18}$$

where T_1 and T_2 are defined by Equations C.10 and C.11, respectively, when $v_1^b = v_1 = v_2$. Equation C.18 implies limits of integration on t_d because $t_d \ge t_c$. Equations C.16 and C.17 are lines with the same slope v_1

Condition 1 $(v_1 = v_2)$ corresponding to Equation C.18 is examined first. If $T_2 \leq 0$, there is no contribution to good block k (i.e., the travel time to block k is greater than Δt). Pocalling that $T_1 \leq T_2 \leq \Delta t$, Figure C.3 shows the only possible interjections of the lines defined by Equation C.18 with the shaded ar a slown in Figure C.2.





Condition 1 $(v_1 = v_2)$ corresponding to Equation C.18 is examined first. If $T_2 \leq 0$, there is no contribution to grid block k (i.e., the travel time to block k is greater than Δt). Recalling that $T_1 \leq T_2 \leq \Delta t$, Figure C.3 shows the only possible intersections of the lines defined by Equation C.18 with the shaded area shown in Figure C.2.

The shaded triangular regions have integration limits

 $T_{d_1} = 0, \quad T_{c_1} = 0$ $T_{d_2} = t_2, \quad T_{c_2} = t_d$ for $t_1 \le 0$

C - 8

$$\begin{bmatrix} T_{d_{1}} & = t_{1}, & T_{c_{1}} & = t_{1} \\ \\ T_{d_{2}} & = t_{2}, & T_{c_{2}} & = t_{d} \end{bmatrix}$$
 for $t_{1} \ge 0$

In either case, $(t_1 \le 0 \text{ or } t_1 \ge))$, Equation C.14 is solved as the sum of the integral evaluated over the triangular region and the integral evaluated over the rectangular region.

Condition 2 $(\nu_1 > \nu_2)$ involves only Equation C.16 and is separated into the following subcases:

Subcase 2.1 $v_1 > v_2 > 0$ Subcase 2.2 $v_1 > 0 > v_2$ Subcase 2.3 $0 > v_1 > v_2$

<u>Subcase 2.1</u> $v_1 > v_2 > 0$

If one writes $t_d = mt_c + B$ then

$$mt_{a} + B_{1} \le t_{d} \le mt_{a} + B_{2} \tag{C.19}$$

alle at

for
$$m = \frac{v_1}{v_1 - v_2}$$
, $B_1 = \frac{k\Delta x - v_2\Delta t}{v_1 - v_2}$, and $B_2 = \frac{(k+1)\Delta x - v_2\Delta t}{v_1 - v_2}$

This subcase therefore has

m > 1 $B_2 > B_1$ $B_1 < \Delta t$ $T_1^* > T_2^*$ $T_2^* < \Delta t$ $k \ge 0$ (C.20)

where (T_1^*, T_1^*) and (T_2^*, T_2^*) are the points of intersection of lines $t_d = mt_c + B_1$, and $t_d = mt_c + B_2$ with line $t_d = t_c$, respectively. That is,

$$T_1^* = \Delta t - \frac{k\Delta x}{v_2}$$

(C.21)

$$T_2^* = \Delta t - \frac{(k+1)\Delta x}{v_2} = T_1^* - \frac{\Delta x}{v_2}$$

The restrictions $k\geq 0$, $T_2*<\Delta t$, $T_1*>T_2*$, $B_2>B_1$, and m>1 follow directly from $v_1>v_2>0$. The restriction $B_1<\Delta t$ can be seen graphically to require a nonzero area of intersection. Algebraically, if

 $B_1 \ge \Delta t$ (C.22)

then

$$\frac{k\Delta x + v_2 \Delta t}{v_1 - v_2} \ge \Delta t \tag{C.23}$$

or

$$k\Delta x \ge v_1 \Delta t$$
 (C.24)

This implies that the distance to the nearest edge of grid block k is longer than the distance a particle can possibly travel. That is, suppose a particle exits the cell at the earliest possible time, $t_c = 0$. Then, migrating during the entire time Δt at the fastest velocity, V_i , (which assumes $t_d = \Delta t$) results in the maximum distance $v_1 \Delta t$.

Figure C.4 shows the 6 possible regions of integration for subcase 2.1. The limits of integration for the subregions of each region are given in Table C.1. Lines L_1 and L_2 denote

L₁:
$$t_d = mt_c + B_1 \text{ or } t_c = 1/m(t_d - B_1)$$

L₂: $t_d = mt_c + B_2 \text{ or } t_c = 1/m(t_d - B_2)$













Figure C.4. The Possible Regions of Integration for Subcase 2.1

Table C.1.

Graph		Regi	on 1		1	Regio	n 2		Region 3				
	T d	Td2	T ° 1	тс2	T d	Td2	т с ₁	т _с 2	T d	Td2	т с 1	т с ₂	
(i)	B	∆t	0	L_1		N/A				N/A			
(11)	B	B 2	0	L_1	B 2	Δt	L ₂	L_1		N/A			
(111)	0	т_*	0	t d	т_*	∆t	0	L_1		N/A			
(iv)	0	т_*	0	td	Т_*	B 2	0	L ₁	B2	Δt	L_2	L_1	
(v)	0	в 2	0	td	в 2	т_*	L ₂	td	T *	Λt	L 2	L_1	
(v1)	T *	т_*	L 2	td	T *	∆t	2	L_1		N/A			

Integration Limits Needed to Evaluate Equation C.14 for Subcase 2.1

The final integration for a region is a sum of integrals over its sub-region.

Subcase 2,2 $v_1 > 0 > v_2$

This subcase is restricted to

0 < m < 1 $T_2^* > T_1^*$ $T_1^* \ge \Delta t$ $\Delta t > B_1 > 0$ $T_2^* < \Delta t$ $\Delta t > B_2 > 0$

(C.25)

 $k \ge 0$

k < 0

The Real Property of

C-12

 $T_1^* > \Delta t$ and $B_1 > 0$ follow from $v_2 < 0$ and $k \ge 0$. $T_2^* < \Delta t$ and $B_2 < \Delta t$ follow from $v_2 < 0$ and $k \le -1$. Intercept B_1 is less than Δt from the travel time required to the nearest edge of grid block k. Intercept B_2 is greater than zero for the same reason.

Figure C.5 shows the 4 possible regions for subcase 2.2. Table C.2 licts the limits of integration by subregion.

Table C.2.

Integration Limits Needed to Evaluate Equation C.14 for Subcase 2.2

Graph	-	Regi	on 1			Regio	n 2		Region 3			
	T d 1	Td2	T c 1	T c 2	T d	T d 2	т _с 1	1 c 2	T d 1	Td2	T c 1	T c 2
(i)	B ₁	Δt	0	td		N/A				N/A		
(i1)	B	B2	0	L l	в 2	۵t	L ₂	L		N/A		
(111)	B	T_*	0	L	т_*	в 2	0	td	B 2	T_*	L_2	t d
(iv)	0	в 2	0	t d	B 2	т_*	L ₂	t d		N/A		

<u>Subcase 2.3</u> $0 > v_1 > v_2$

Since both velocities are negative, particles in these bins must travel in a negative direction. Thus, only $k\leq$ -1 is allowed. The following restrictions apply.

$$\left. \begin{array}{c} m < 0 \\ B_2 > B_1 \\ B_2 > 0 \\ T_1^* < \Delta t \\ T_2^* < \Delta t \end{array} \right\}$$
 (C.26)







Figure C.5. Regions of Integration for Subcase 2.2

 $m < 0, \ B_2 > B_1, \ T_1 \star < \Delta t, \ and \ T_2 \star < \Delta t \ follow \ from \ k \le -1, \ v_2 \le 0, \ and \ v_1 - v_2 > 0.$ Intercept B_2 is positive because the minimal travel time to the nearest edge of block k must be less than $\Delta t.$

Figure C.6 shows the 7 possible regions for subcase 2.3. Table C.3 lists the corresponding limits of integration by subregion.

The 17 regions of subcases 2.1 to 2.3 completely describe the integration limits for condition 2 $(v_1 > v_2)$. The limits for condition 3 $(v_2 > v_1)$ are the same if the roles of lines L_1 and L_2 are reversed. Thus, defining

Subcase 3.1 $v_2 > v_1 > 0$ Subcase 3.2 $v_2 > 0 > v_1$ Subcase 3.3 $0 > v_2 > v_1$

one has the correspondences

Subcase	3.1			*>	Subcase	2.3		
Subcase	3.2	(k ≥	: 0)	€ +	Subcase	2.2	(k ≰	-1)
Subcase	3.2	(k ±	-1)	+>	Subcase	2.2	(k ≥	0)
Subcase	3.3			*+	Subcase	2.1		

Returning to Equation C.14, it can be rewritten as

$$pr(2,1,k,b) = K_{a} \int_{T_{d_{1}}}^{T_{d_{2}}} e^{-(\lambda_{1} - \lambda_{2})t_{d}} \left[\int_{T_{c_{1}}}^{T_{c_{2}}} e^{\lambda_{1}t_{c}} dt_{c} \right] dt_{d}$$

$$= \frac{K_{a}}{\lambda_{1}} \int_{T_{d_{1}}}^{T_{d_{2}}} e^{-(\lambda_{1} - \lambda_{2})t_{d}} \left[e^{\lambda_{1} T_{c_{2}}} - e^{\lambda_{1}T_{c_{1}}} \right] dt_{d}$$
(C.27)



Figure C.6. Regions of Integration for Subcase 2.3

Table C.3.

Graph		Regio	n 1			Regio	n 2		Region 3				
	T d 1	T d 2	т _с 1	T C 2	T d	T d 2	T C 1	т _с 2	τ d 1	T d 2	т с 1	т _с 2	
(i)	0	T_*	0	td	T_*	B 2	0	L ₂		N/A			
(11)	0	T_*	0	td	T_*	Δt	0	L ₂		N/A			
(iix)	T_*	т ₂ *	L_1	td	т_*	B 1	L ₁	L_2	в 1	в 2	0	L_2	
(iv)	T_*	B 1	L ₁	td	B 1	т_*	0	td	т_*	B 2	0	L ₂	
(v)	T_*	B 1	L	td	B 1	T_*	0	td	T_*	Δt	0	L ₂	
(vi)	T *	1,*	L ₁	td	т_*	B 1	L_1	L_2	B 1	Δt	0	L ₂	
(vii)	T_*	т_*	L ₁	td	T_*	Δt	L	L ₂		N/A			

Integration Limits Needed to Evaluate Equation C.14 for Subcase 2.3

where $K_a = \frac{h_{1,2}\lambda_1 e}{\Delta t N_{y}}$. From the above conditions, it is known that T_{c_1} and T_{c_2} are linear functions of t_d . In general, one can write

$$T_{c_1} = \alpha_1 t_d - \beta_1$$

$$T_{c_2} = \alpha_2 t_d - \beta_2$$

(C.28)

•

Equation C.27 Lecomes

$$pr(2,1,b,k) = \frac{K_{a}}{\lambda_{1}} \int_{T_{d_{1}}}^{T_{d_{2}}} \left[e^{-(\lambda_{1}(1 - a_{2}) - \lambda_{2})t_{d}} e^{-\lambda_{1}\beta_{d}} e^{-\lambda_{1}\beta_{d}} e^{-(\lambda_{1}(1 - a_{1}) - \lambda_{2})t_{d}} e^{-\lambda_{1}\beta_{1}} e^{-\lambda_{$$

$$=\frac{\kappa_{e}}{\lambda_{1}} e^{-\lambda_{1}\beta_{2}} \left[\frac{e^{-(\lambda_{1}(1-\alpha_{2})-\lambda_{2})T}d_{1} - (\lambda_{1}(1-\alpha_{2})-\lambda_{2})T}d_{2}}{\lambda_{1}(1-\alpha_{2})-\lambda_{2}} - \frac{(\lambda_{1}(1-\alpha_{2})-\lambda_{2})T}d_{2}}{\lambda_{1}(1-\alpha_{2})-\lambda_{2}} \right]$$

$$-e^{-\lambda_1\beta_1} \begin{bmatrix} \cdot(\lambda_1(1-\alpha_1)-\lambda_2)T_{d_1} & \cdot(\lambda_1(1-\alpha_1)-\lambda_2)T_{d_2} \\ e & -e & \\ \hline & \lambda_1(1-\alpha_1)-\lambda_2 \end{bmatrix}$$

$$=\frac{h_{1,2}}{\Delta t N_{y}} \left\{ \frac{e^{-\lambda_{1}T_{21}}e^{-\lambda_{2}(\Delta t - T_{d_{1}})} - e^{-\lambda_{1}T_{22}}e^{-\lambda_{2}(\Delta t - T_{d_{2}})}}{\lambda_{1}(1 - \alpha_{2}) - \lambda_{2}} \right\}$$

$$\frac{e^{-\lambda_{1}T_{11}}e^{-\lambda_{2}(\Delta t - T_{d_{1}})} - e^{-\lambda_{1}T_{12}}e^{-\lambda_{2}(\Delta t - T_{d_{2}})}}{\lambda_{1}(1 - \alpha_{1}) - \lambda_{2}} \right] \qquad (C.29)$$

5

where

$$T_{rp} = (1 - \alpha_r)T_{d_p} + \beta_r$$
 $r, p = 1, 2$. (C.30)

The above integration is valid as long as $\lambda_1(1+\alpha_r)-\lambda_2\neq 0$. The possible values for α_r are

$$\alpha_{r} = 0$$

 $\alpha_{r} = 1$
 $\alpha_{r} = 1/m = \frac{v_{1} - v_{2}}{v_{1}}$
(C.31)

If $\alpha_r = 0$, $\lambda_1 \neq \lambda_2$ is required; If $\alpha_r = 1$, $\lambda_2 \neq 3$; and if $\alpha_r = 1/m$.

$$\frac{\lambda_1}{\lambda_2} \neq \frac{v_1}{v_2}$$

If λ_1 (1 - α_r) - λ_2 = 0 for any case. Equation C.29 is replaced by

$$pr(2,1,b,k) = \frac{h_{1,2}}{\Delta t N_{1}} e^{-\lambda} 1^{\beta} r e^{-\lambda} 2^{\Delta t} (T_{d_2} - T_{d_1})$$

Finally, $\mathbb{T}_{rp} \ge 0$ since

 $t_c = \alpha_r t_d - \beta_r$

implies

$$t_d - t_c = (1 - \alpha_r)t_d + \beta_r \qquad (C.32)$$

for all values of $t_{\rm d},$ and the left hand side of Equation 0.32 is non-negative. In fact

$$T_{rp} = T_{dp} - T_{cr}; r.y = 1,2$$
 (C.33)

The final step in finding $S_{\rm F}$ is to sum over velocity bins for each block $k_{\rm c}$

$$S_{F}^{(2,1,k)} = \sum_{b}^{N_{V}} pr(2,1,k,b)$$
 (C.34)

Here, pr(2, 1, k, b) = 0 if

$$\Delta t \max \left\{ v_1^b , v_2^b \right\} \leq k \Delta x \; ; \; k \geq 0$$

$$\Delta t \min \left\{ v_1^b , v_2^n \right\} \geq (k + 1) \Delta x \; ; \; k \leq -1 .$$

$$(C.33)$$

In factice, the entries $S_F(2,1,k)$ may be positive but negligible for some extreme values of k.

The last case (j > 1) involves decay chains of length greater than two. To implement the algorithm, a simplifying assumption is made. For the chain

 $i \rightarrow P_i \rightarrow i \rightarrow P_i + 1 \rightarrow \dots \rightarrow i \rightarrow i \rightarrow i$,

if a source particle of species type i-j (for some j, $2 \le j \le P_i$) crosses the cell boundary at t_e and is of species type i at the end of Δt , the decay from species i-j to species i-l is assumed to be single process. During this decay process, the particle travel, with a velocity that is an arithmetic average of the velocities assigned to species i-j,...i-l.

The average velocity for the velocity bin b is

$$v^{b} = \frac{1}{j} \sum_{\substack{i=1 \\ j \neq i}}^{J} v^{b}_{i-j},$$
 (C.36)

There are five probabilities similar to the case j=1.

 The probability that an atom of species i-j exits the cell during time dt, about t, is

C-20

2. The probability that an atom of species 1-j decays to species 1-1 during time $t_d + t_c$ is

$$\sum_{n=2}^{j} h_{i+n;i+n+1} \lambda_{i+n} \sum_{\ell=2}^{j} \frac{e^{-\lambda_{i-\ell}(t_d - t_c)} - e^{-\lambda_{i-1}(t_d - t_c)}}{\prod_{\substack{m=1\\m \neq \ell}} (\lambda_{i-m} - \lambda_{i-\ell})}$$

 The probability that an atom of species 1-1 decays to species 1 curing dt_d about t_d is

h_{i-1,i} ¹_{i-1}dt_d

4. The probability that an atom species i survives decay from $t_{\rm d}$ to Δt is

 $e^{-\lambda}i (\Delta t - t_d)$

5. The probability that an atom 1 assigned to velocity bin b is $1/N_{\nu}$. Similar to j=1, it is ass med that the particles maintain the same velocity bin over Δt as they decay.

The probability that a source particle of type $i \cdot j$ ends Δt occupying grid block k as type i is

$$pr(i-j,i,k,b) = \frac{h_{i-1,i}\lambda_{i-1}}{N_{v}\Delta t} \prod_{n=2}^{n} h_{i-n,i+n+1}g_{i-n}e^{-\lambda \Delta t}$$
(C.37)

$$\int_{T_{d_1}}^{T_{d_2}} \int_{t_{c_1}}^{T_{c_2}} e^{-\lambda_1 t_d} \int_{\ell=2}^{\frac{j}{\Sigma}} \frac{e^{-\lambda_{1-\ell}(t_d - t_c)} - e^{-\lambda_{1-1}(t_d - t_c)}}{\prod_{\substack{m=1\\m\neq\ell}}^{j} (\lambda_{1-m} - \lambda_{1-\ell})} dt_c dt_d$$

where ${\rm T}_{d_1},~{\rm T}_{d_2},~{\rm T}_{c_1},~{\rm T}_{c_2}$ are determined as in the case j=1 with v_i

replacing v_2 and \overline{v}^b (Equation C.36) replacing v_1 . In particular, recall that t_c is a linear function of t_d and
$$T_{c_1} = \alpha_1 t_d + \beta_1$$

$$T_{c_2} = \alpha_2 t_d + \beta_2$$
(C.38)

The details of solving Equation C.37 are omitted except for noting the use of the identity



in der to combine terms following the integration.

Thus,

$$pr(i-j,i,k,b) = \frac{1}{N_{v}\Delta t} \prod_{n=1}^{J} h_{i-n,i-n+1}\lambda_{i-n}$$

$$\int_{\mathcal{L}} \left\{ \begin{bmatrix} j \\ \Pi \\ m=1 \\ m \neq \ell \end{bmatrix} (\lambda_{i-m} \cdot \lambda_{i-\ell})^{-1} \right] \frac{1}{\lambda_{i-\ell}}$$
(C.39)

$$\frac{\left[e^{-\lambda_{1}}\cdot\ell^{T}_{22}e^{-\lambda_{1}}\left(\Delta t + T_{d_{2}}\right) - e^{-\lambda_{1}}\cdot\ell^{T}_{21}e^{-\lambda_{1}}\left(\Delta t - T_{d_{1}}\right)\right]}{\lambda_{1} + \lambda_{1}\cdot\ell^{-(1-\alpha_{1})}}$$

$$\frac{e^{-\lambda_{i \cdot \ell} T_{12}} e^{-\lambda_{i} (\Delta t \cdot T_{d_{2}})} e^{-\lambda_{i \cdot \ell} T_{11}} e^{-\lambda_{i} (\Delta t \cdot T_{d_{1}})}}{\lambda_{i} \cdot \lambda_{i \cdot \ell} (1 \cdot \alpha_{1})} \right]$$

where the $T_{\rm rp}$ (r,p=1,2) are defined by Equation C.30. The restrictions of nonzero denominators still apply and if zero denominators are detected the term

 $e^{-\lambda_1 \Delta t} e^{-\lambda_1 \cdot \ell \beta_r} (T_{d_2} \cdot T_{d_1})$

replaces

$$\frac{e^{-\lambda_{1-l}T_{rp}}e^{-\lambda_{\lambda}(\Delta t - T_{dp})}}{\lambda_{1} - \lambda_{1-l}(1 - \alpha_{r})}$$

The conditions stated in Equation C.35 apply to set pr(i-j,i,k,b) = 0 for blocks k that do not receive source particles. Collecting fractions over velocity intervals then yields

$$S_{F}(i, i \cdot j, k) = \sum_{b=1}^{N_{V}} pr(i \cdot j, i, k, b)$$
 (C.40)

Equation C.40 must be generated for each parent 1-j, j=2, ..., P_1 .

Finally, defining

$$\prod_{\substack{m=1\\m\neq\ell}}^{j} (\lambda_{i-m} - \lambda_{i-\ell}) = 1$$
 (C.41)

for the case $\ell=j=1$, Equation C.39 will contain Equation C.29. Thus, Equations C.13 and C.40 can be used to completely define S_F .



APPENDIX D

Storage of Decay Chain Information

The storage of decay chain information in NEFTRAN II is presented in this appendix, first for the case where no branches occur in the decay chain, and next for the case where branches are present in the chain. The subroutine BRANCH is then discussed in terms of arrays presented in the first two discussions.

I. Decay Chain Without Branching

П

Example: $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5$

NEFTRAN potentially transports $\frac{5(5+1)}{2}$ = 15

L	1	-4	1				8.	3	-18	4					
2	2	×.	2				9.	2	18	3	-6	4			
3	1	÷,	2				10.	1	$\sim 10^{-10}$	2	-4	3		4	
4.4	3	-10	3				11.	5	-0	5					
5.	2	÷ŝ.	3				12.	4		5					
5.	1	÷	2	$\cdot \sigma$	3		13.	3	-4	4	-14	5			
7 .	4	18.	4				14.	2	$\rightarrow 3$	3	-18	4	~ 4	5	
							15.	1	-16	2	vik	3		4	 5

Howeve, Subroutine BRANCH may determine that some of the longer subchains are not necessary. That is, the contribution to species 5 from the decay of species 1 over a time step \$t, may be insignificant.

If BRANCH decides that all are necessary, then define the LPS (loop start) and LPE (loop end) arrays for each species as follows:

LPS(1)	-	1	LPE(1)		1
LPS(2)	-	2	LPE(2)	-	3
LPS(3)	-	4	LPE(3)	-	6
LPS(4)	-	7	LPE(4)	-	10
LPS(5)	-	11	LPE(5)		15

If the subchains above were numbered 1-15, then those ending with species I are found from

LPS(I) to LPE(I).

The arrays LPS and LPE are used to define end points of DO-loops.

DO 20 I=1, NOISO J1 = LPS(I) J2 = LPE(I) DO 10 J = J1, J2

D-1

This type of loop occurs throughout NEFTRAN II.

In such a loop, variable J is normally used to retrieve information about subchain J. Subchains are defined by the LRP-array.

LRP(1,1)	-	1	LRP(7,1) = 4
LRP(1,2)	-	1	LRP(7,2) = 1
			LRP(8,1) = 3
LRP(2.1)	-	2	LRP(8,2) = 2
LRP(2.2)		1	LRP(9,1) = 2
IRP(3.1)		i.	LRP(9,2) = 3
1.RP(3.2)		2	LRP(10,1) = 1
care (a i mi		÷.	LRP(10, 2) = 4
LRP(4,1)	÷	3	
LRP(4.2)	-	1	· · · ·
LRP(5,1)	-	2	
LRP(5,2)	146	2	
LRP(6.1)		1	
LRP(6,2)	*	3	

For species I, look in LRP array from

LPS(I) to LPE(I).

For LPS(I) $\leq J \leq$ LPE(I), subchain J has LRP(J,1) members and the first member is species LRP(J,1).

Example: I = 3, $4 \le J \le 6$. If J = 6, then subchain 6 has length LRP(6,2) = 3 and the top member of the chain is LRP(6,1) = 1.

If Ecanches were not allowed, only one column (either one) of LRP would be necessary. In fact, LRP could probably be done away with. Its necessity will be demonstrated in Section II.

Application. Consider the DP-array, which contains decay and production fractions for each subchain over a time step. That is,

DP(1) - fraction of 1 surviving decay over Δt DP(2) - fraction of 2 surviving decay over Δt DP(3) - fraction of 1 that decays to 2 (and no farther) over Δt DP(4) - fraction of 3 surviving decay over Δt DP(5) - fraction of 2 that decays to 3 (and no farther) over Δt DP(6) - fraction of 1 that decays to 3 (and no farther) over Δt •

So, to update an inventory for species 3, treat all subchains ending in 3, which can be found between LPS(3) and LPE(3).

SUM = 0 JI = LPS(3) J2 = LPE(3)

Variable SUM will contain the inventory of species 3 after a time step At, where the atoms array contains inventories of all species at time 0.

There are several other arrays in NEFTRAN which rely on the pointers LPS and LPE. All such arrays are dimensioned to the maximum number of subchains (+1 for some).

(14, JV, V, N, JF, JSF, INSR, JPSC)

II. Decay Chain With Franching.



The possible subchains are:

Example:

1. 2. 3. 5. 6. 7. 8.	$1 \rightarrow 1$ $2 \rightarrow 2$ $1 \rightarrow 2$ $3 \rightarrow 3$ $1 \rightarrow 3$ $4 \rightarrow 4$ $2 \rightarrow 4$ $1 \rightarrow 2 \rightarrow 4$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	- 4 - 5 - 4 - 5 - 5 - 4 - 5
	LRP Col. 1	LRP Col. 2	
1	1	11111	LPS(1) = 1, LPE(1) = 1
2	2	2. The P. S. S.	LPS(2) = 2, $LPE(2) = 3$
3		2	
4		1	LPS(3) = 4, $LPE(3) = 5$
5	1	2	
6		1	LPS(4) = 6, $LPE(4) = 10$
7	[사다. 2 관계 관계 전 관리 다 ?	2	
8		3	
9		2	
10	1	3	
n.	10일은 전 것이다.	1	LPS(5) = 11, LPE(5) = 16
12	4	2	
	1. 2. 3. 4. 5. 6. 7. 8. 1 2. 3. 4. 5. 6. 7. 8. 1 2. 3. 4. 5. 6. 7. 8. 1 2. 3. 4. 5. 6. 7. 8. 10 11. 12. 10 11. 12. 10 10 11. 12. 10 10 11. 12. 10 10 10 10 10 10 10 10 10 10 10 10 10	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1. 1 + 1 9. $3 \div 4$ 2. 2 $\div 2$ 10. $1 \Rightarrow 3$ 3. $1 \div 2$ 11. $5 \Rightarrow 5$ 4. $3 \div 3$ 12. $4 \Rightarrow 5$ 5. $1 \Rightarrow 3$ 13. $2 \Rightarrow 4$ 6. $4 \Rightarrow 4$ 14. $1 \Rightarrow 2$ 7. $2 \Rightarrow 4$ 15. $3 \Rightarrow 4$ 8. $1 \Rightarrow 2 \Rightarrow 4$ 16. $1 \Rightarrow 3$ 1 1 1 1 2. 2 1 3 3. 1 2 1 4 3 1 2 4 3 1 2 4 3 1 2 6 4 1 2 8 1 2 3 9 3 2 3 9 3 2 3 10 1 3 3 2 2 2 3 9 3 2 3 9 3 2 3 <

row 13	2	3
row 14	1	4
row 15	3	3
row 16	1	4

Note that row 8 is the same as row 10 and row 14 is the same as row 16. However, the information in row 8 in arrays B, JV, ... is for subchain #8, not #10.

There are places in the code, however, where this does present a problem. For example, if the subchain ends in species 4, is of length 3, and has ultimate parent 1; what is the identity of the intermediate species?

 $1 \rightarrow 2 \rightarrow 4$ or $1 \rightarrow 3 \rightarrow 4$?

The intermediate species identity must be known for finding discharge factors. Two velocities are required $v_4 \& v_1$, or $v_4 \& v_{1 \to 3}$

Examining subroutine SETDIS:

$1 \rightarrow 2 \rightarrow 4$ KP = 8	ISV = 2 ISP = 1 find 1 → 2,	IJ = LPS(2), LPE(3) = 2,3 ISL = LT-1 = 2 KS = 3	
$1 \rightarrow 3 \rightarrow 4$ KP = 10	ISV = 3 ISP = 1 find 1 → 3	IJ = 4,5 ISL = 2 KS = 5	
4 → 5	ISV = 4		
$2 \rightarrow 4 \rightarrow 5$ KP = 13	$IJ = 6,10$ find 2 $\rightarrow 4$	ISP = 2 ISL = 2 KS = 6	
$1 \rightarrow 2 \rightarrow 4 \rightarrow 5$ KP = 14	$\begin{array}{ll} \text{IJ} = 8,10\\ \text{find} \ 1 \rightarrow 2 \rightarrow 4 \end{array}$	ISP = 1 ISL = 3 KS = 8	
$3 \rightarrow 4 \rightarrow 5$ KP = 15	$\begin{array}{l} 1J = 9,10\\ \text{find } 3 \rightarrow 4 \end{array}$	ISP = 3 ISL = 2 KS = 9	
$1 \rightarrow 3 \rightarrow 4 \rightarrow 5$ KP = 16	IJ = 10, 10 find 1 - 3 - 4	ISP = 1 ISL = 3 KS = 10	

Treating/Locating Branching Fractions

 $1 \rightarrow 2 \text{ at } .3$ $1 \rightarrow 3 \text{ at } .7$

On input: Iso 2 par = 1 frac = .3 Iso 3 par = 1 frac = .7 In CHAIN: 1FR BRFR 1. \$ 2 3 0. .7 .7 2. 0 0. 3. 0 0. 4. 0 0. 5. 0 0. In SETDIS: 1 - 2 GO TO 80 W/KM = 1 If (3 .eq. 2) 7 KP = 3 since \neq , BFR = 1 · BFR = 1 LT = 2 - .7 - .3 1 + 3 GO TO 80 w/KM = 1 If (3 .eq. 3) ? KP = 5 since ≠, BFR ⊷ .7 (remains) LT = 2 3 - 4 2,9 is 1 = LRP(7,...,0, 2)LKP = 1 KP = 9find at 6, 2M = 3 LT = 2If (0 .eq. 1) since # BFR = 1 - BRR = 1. 1 - 2 - 4 GO TO 80 w/KM = 1 If (3 .eq. 2) KP = 8no BFR = 1 - .7 = .3 LT = 3 $1 \rightarrow 3 \rightarrow 4$ GO TO 80 W/KM = 1 If (3 .eq. 3) KP = 10 BFR = .7 LT = 3

<u>Subroutine BRANCH</u>. In either case presented above, it may not be necessary to transport all subchains.

Example: $1 \rightarrow 2 \rightarrow 3 \rightarrow 4$

 $T^{1/2}(1) = 10y$ $T^{1/2}(2) = 50y$ $T^{1/2}(3) = 10^4y$ $T^{1/2}(4) = 100y$

The production of iso #4 by isos #1 and #2 might be insignificant compared to the production by #3 over a time step.

So, it is not necessary to transport subchains

1 - 2 - 3 - 4 nor 2 - 3 - 4

In addition to setting up LPS, LPE, LRP, and DF, BRANCH decides necessary subchains. User can force all subchains by setting EPS = 0 in argument list (code change). Branch is called by SOURCE (update inventory to TRLSE), DTUPDT (age inventory by Δt -source), SETUP (age inventory by Δt -transport), with EPS = 10^{-8} , 10^{-4} .

Branch looks at all paths from daughter iso IR to the end(s) of the chain. Can be up to 4 paths.



Branch finds 2 paths $1 \rightarrow 2 \rightarrow 4 \rightarrow 5$ $1 \rightarrow 3 \rightarrow 4 \rightarrow 5$

and will store in array IW.

The coding that is implemented for this example is as follows:

IR = 5 NB = 0 (# brand pts detected)
 NP = 1 (# paths)
 KR = IR = 5
 I = 1
 IW(1,1) = 5

10 Loop

I = 2 IW(1,2) = 4 no 2nd parent KR = 4 I = 3 IW(1,3) = 2 yes 2nd parent IPAR(4,1) = -2 NB = 1 KR = 2 KR = 1

I = 4 IW(1,4) = 1 no 2nd parent hit end of chain, go to 30

40 Loop

Detect IPAR(4,1) = -2 (<0) Set IPAR(4,1) = 2 & go to 50 50 NP = 2 60 Loop K = 1, 1⁽⁴⁾

If $(IW(1,K) = J^{(4)})$ go to 70 true for K = 2

70 1 - 3 IW(2,1) = IW(1,1) 5 IW(2,2) = IW(1,2) 4 KR = 3 IW(2,3) = 3 NB = 010 Loop I = 4 IW(2,4) = 1 no 2nd parent KR = 1 hit end of chain, go to 30 30 NB - 0 so go to 100 At this point: IW(1,1) = 5IW(1,2) = 4IW(1,3) = 2IW(2,1) # 5 IW(2,2) = 4IW(2,3) = 3IW(1,4) = 1IW(2,4) = 1At 100 - 200 IS = 2 ISD = 2 LPS(5) = LPE(4) + 1LT = LPS(5)LRP(LT,1) = 5LRP(LT, 2) = 1 $DP = e^{-\lambda\Delta t}$

 $D(2) = \lambda_4$ define branch frac = 1. LT = LT + 1 (stacking in LRP, DP) $DP(LT) = prod 1 \rightarrow 2 \text{ over } \Delta t$.

APPENDIX E

Output Files for Sample Problems

NEFTRAN 11 - PC VERSION RELEASED OCTOBER 1990

NEFTRAN II: SAMPLE PROBLEM #1 FOR USER'S MANUAL (PC VERSION) EXECUTION DATE 11/12/1990 AND TIME 12: 7:40

4

PARAMETERS

GROUP1 - OPTIONS

.

STAN	DARD P	RINT, NONZERO #> PRINT	
PTION	VALUE	OUTPUT-DESCRIPTION	
1	1	LIST OF ALL PARAMETERS	
2	1	THE WETWORK LEG PROPERTIES ARRAY	
3	1	THE VETWORK JUNCTION PROPERTIES ARRAY	
4	1	THE MIGRATION PATH PROPERTIES ARRAY	
5	1	THE DECAY CHAIN PROPERTIES ARRAY	
6	1	THE ELEMENT PROPERTIES ARRAY	
7	1	FLUID VELOCITIES & SOURCE/DISCH FLOWRATES	
8	0	SUBCHAINS- DECAY, PRODUCTION, & VELOCITIES	
9	0	SPACE & TIME STEPS AND SOURCE TYPE	
10	1	TIME DEPENDENT OUTPUT	
		- IF +N, DISCHARGE RATES EVERY NTH TIME STEP	
		- 1F -N, CONCENTRATIONS EVERY NTH TIME STEP	
11	1.1	D'SCHARGE SUMMARY	
EXTE	RNAL	FILES, NONZERO >> FILE WRITTEN/READ	
OPTION	VALUE	CORRESPONDING FILE	
12	0	WRITE SRATE.DAT, SOURCE RATES (CI/y)	
13	1	WRITE DRATE.DAT, DISCHARGE RATES (C1/Y)	
14	0	NOT CURRENTLY USED	
15	0	READ SAMP.DAT, SAMPLED DATA NORMALLY FOR REPEATE?	RIALS
16	0	READ VFIELD.DAT, TIME DEPENDENT VELOCITIES	
17	0	READ SFLOW, DAT, TIME DEPENDENT FLOWRATES	
21.16	CONTR	0.8	
DOTION.	VALUE	DECODIDIIN	
10	THELE	USE DUNION OF ANALYTIC SOLN(1)	
10		COLVE NETWORKING OR INDUT VELOCITIES(1)	
20	0	LEADWIDS SOLUEILITIES(1) OF BOTH(2)	
21		ELOUTHRIJON MINCELLIN DR CHENSE(2)	
22	6	CONSTANTION OF EXPONENTIAL (1) LEACH RATE	
23	ñ	FORCE(1) USE OF LEG-TO-LEG TRANSFER ALGORITHM	
6.0		CRUERS IN AND ALL PER IN TER INTERIOUS ADDRESS OF	

DEBUG PRINTS, NONZERO => PRINT OPTION VALUE OUTPUT-DESCRIPTION

-9

Û

24	0	DVM MULTIPLIERS F	OR TRANSPORT,	DISCHARGE,	AND SOURCE
-25	0	DIAGNOSTIC INFO F	OR SUBROUTINE	BAND	

26	0	DIADNOSTIC 18FO FOR FUNCTION OIT
27	0	MATRIX/VECTOR SYSTEM TO BE SOLVED FOR FLOW
28	0	THE DATA FROM UNIT 10, SAMP.DAT
29	0	NOT CURRENTLY USED
30	0	INVENTORY AT RELEASE TIME
31	0	RESTRICTIONS PLACED ON THE TIME STEPS
32	1	LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
33	0	VELOCITIES FROM THE EXTERNAL FILE, UNIT 11
34	0	THE ATOM COUNT SUMMARY
35	1	JUNCTION PRESSURES & LEG FLOWRATES
36	0	LEG-TO-LEG TRANSFER FRACTIONS
37	0	TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN
38	0	TIME DEPENDENT SOURCE FLOWRATES

GROUP2 - PROBLEM SIZES

VALUE	DESCRI	PTIC	N N	
16	NUMBER	3F	NETWORK LEGS	
13	NUMBER	OF	NETWORK JUNCTIONS	
5	NUMBER	OF	MIGRATION PATH LECS	
- 3 - C	NUMBER	OF	DECAY CHAINS INPUT	
3	NUMBER	OF	ELEMENTS INPUT	
			DECAY	CHAINS
			NUMBER	NCLUS

NUMBER INCLUSION MEMBERS INDEX 3 D

GROUP3 - SOURCE/FLOW PARAMETERS

VALUE 1.0000E+00	DESCRIPTION FRACTION OF SOURCE ACCESSED
0.0000E+00	PORE VOLUME CONTAINING SOURCE (ft**3)
0.0000E+00	FORE-AREA FOR SOURCE REGIME (ft**2)
1.0000E-05	LEACH RATE (1/y)
0.0000E+00	DEJSITY OF SOURCE FLUID (16/ft**3)
0.0000E+00	PORE-AREA AT DISCHARGE (ft**2)

GROUP4 - TIME PARAMETERS

VALUE	CESCRIPTION
1.00005+06	TIME TO END OF SIMULATION (Y)
0,0000E+00	TIME OF ONSET OF MIGRATION (y)
0.00000400	TIME OF ONSET OF LEACHING (Y)
0.000000+00	TIME STEP FOR SCARCE (y)
	TRANSPORT TIME STEPS FOR EACH CHAIN
	CHAIN# TIME STER(y)
	1 0.000E+00

GRCUPS - INCREMENT DETERMINATION

DEFAULT values utilized

Network Properties Array

Lep	Inlet	Outles	Length	Area	Hydraulic	Brine
	101	jet	(11)	(sq-ft)	K (ft/d)	Conc.
1	1.1	4	1.450E+05	6.0008+06	5.000E+01	0.000E+00
2	· 4 · ·	5	8.000E+03	6.0008+05	5.000E+01	0.000E+00
3	5	10	3.800E+04	6.000E+06	5.100E+01	0.000E+00
6	10	3	1.0008+05	6.000E+06	5.000E+01	0.000E+00
5	2	9	1.4506+04	1.800E+06	4.000E+01	0.000E+00
6	9	11	8.0008+03	1.800E+06	4.000E+01	0.000E+00
7	11	12	3.800E+04	1.800E+06	4.000E+01	0.000E+00
8	12	13	1.000E+05	1.8008+06	4.000E+01	0.000E+00
9	6	4	6.000E+02	7.070E+02	1.000E-01	6.700E-01
10	8	5	4.965E+02	1.000E+00	1.000E+01	1,000E+00
11	9	6	5.0008+02	1.0008+00	1.670E-06	1.000E+00
12	3.5	8	6.035E+02	1.000E+00	1.509E-06	1.000E+00
13	6	7	4.000E+03	5.4008+02	1.000E+01	1,0008+00
14	7	.8	4.000E+03	5.400E+02	1.0000+01	1.000E+00
15	12	10	1.100E+03	1.0006+00	1.5708-06	1.0000 +00
16	13	3	1,1006+03	1.2008+08	2.5008+00	0.000E+00

	Junction Pri	operties Array		
Jot	Elevation	Known Press?	Pressure	
#	(ft)	No/Yes * 0/1	(psi)	
1	3.602E+03		4.327E+02	
2	2.502E+03	1	6.461E+02	
3	1.526E+03	1	4-327E+02	
4	3.415E+03	0	0.000E+00	
5	3.311E+03	0	0.000E+00	
6	2.8158+03	0	0.000E+00	
7	2.815E+03	0	0,COOE+00	
8	2.8156+03	0	0.000E+00	
0	2.3158+03	0	0,000E+00	
10	2.82GE+03	0	0.000E+00	
11	2.211E+03	0	0.000E+00	
12	1.720E+03	0	0.000E+00	
13	4.2596+02	0	0.0006+00	

Rigration Path Properties Array

Leg	Dispersivity	Space Step	Diffusion?	Mobile	(manob) (e	Mass Xter	Actocità
#	(11)	(ft)	No/Yes=0/1	Porosity	Porosity	Coef (1/y)	(ft/y)
13	5.000E+02	0.0008+00	0	3.000E-D1	0.0001 +00	0.000E+00	0.0002+00
34	0.000E+00	0.000E+00	0	3.00CE -01	0.000E+00	0.000E+00	0.000E+00
10	0.000E+00	0.000E+00	0	1.500E-01	0.000E+00	0.000E+00	0.00000.00
3	D.000E+00	0.000E+00	0	3.0002-01	0.000E+00	0.000E+0J	0.000E+00
4	0.000E+00	0.000E+00	0	3.000E-01	0.000E+00	0.000E+00	0.000E+00

					lecay Chi	ain Array				
Name A6	Atomic Mass	Elem. Index	Local Index	Parent	Parent # 2	Fraction From # 1	Fraction From # 2	Inventory (Ci)	Half-life (y)	Weighting Factor
DECAY NP237 U233 1H229	CHAIN # 1 237.0 233.0 225.0	123	1 2 3	0 1 2	0	0.000E+00 1.000E+00 1.000E+00	0.000E+00 0.000E+00 0.000E+00	1.000E+03 1.000E+03 1.000E+03	2.140E+06 1.620E+05 7.300E+03	1,000E+00 1,000E+00 1,000E+00

	Element Properties Array							
Elem. Index	Solubility (9/9)	Leg #	Mobil Rd	Immobile Rd				
1	0.0008+00	13 14 10 3 4	1.000E+00 1.000E+00 1.000E+00 6.357E+02 6.357E+02	0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.001E+00				
2	0.000E+00	13	1.000E+00 .0/0E+00 .00E+00 .7E+02 357E+02	0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00				
3	0.000€+00	13 14 10 3 4	1,000E+00 1,000E+00 1,000E+00 6,357E+02 6,357E+02	C.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00				

1

THE JL ARRAY JC1 LEGS 1 1 0 0 2 5 0 0 3 -4 -16 0 4 -1 -9 2 5 -2 -10 3 6 -11 9 13 7 -13 14 0 8 -12 -14 10 9 -5 6 11 10 -3 -15 4

~

.

-

S Alter -

11	-6	7	12
12	+7	8	15
13	-8	16	0

PRESSURES AT THE LEG JUNCTIONS

ł

JUNCTION FLUID PRESSURE (ps1)

1	4.3270E+02
2	6.4610E+02
3	4.3270E+02
6	4.3270E+02
5	4.3270E+02
6	7.2025€+02
1	7.19786+02
8	7.1931E+02
9	6.6992E+02
0	4.3270E+02
1	6.8307E+02
2	7.4550E+02
3	9.0980E+02

VOLUMETRIC FLOW RATE FOR EACH LEG LEG FLOW ft**3/y

1	1.4177E+09
2	1.4177E+09
3	1.4177E+09
4	1.4177E+09
5	2.4040E+08
6	2.4040E+08
7	2.4040E+08
8	2.4040E+08
9	-3.7375€+02
10	3.73756+02
11	-6.0667E-04
12	-5.08936-04
13	3.7375E+02
14	3.7375E+02
15	-2.1310E-04
16	2.404CE+08

FOR STEADY-STATE FLOW

EG NO.	PORE VELOCITY
	ft/y
13	2.3071E+00
14	2.3071E+00
10	2.4917E+03
3	7.8759E+02
4	7.8759E+02

PATH LENGTH FROM SOURCE BOUNDARY (ft) = 1.4250E+05AVERAGE FLUID VELOCITY (ft/y) = 7.4637E+01

-

Cast of

FLOW RATE THROUGH BOURCE = 3.7375E+02 ft**3/y FLOW RATE AT DISCHARGE = 1.4177E+09 ft**3/y

RAPIONDELIDE	DISCUNCT	HAIR (CIVI)	
YEAR	NF237	U233	18229
7.52158-04	5.60348-09	5.72158-09	5.7262E-09
7.6973E+04	80-39825.5	2.2850E-08	2.25b9E-08
7.8731E+04	8.01868-08	8.19438-08	8.2013E-08
8.04898+04	2.6000E-07	2.6580E-07	2.66041.07
8.22478+04	7.67671-07	7.85136-07	7.85836-07
8.4006E+04	2.07686-06	2.12498-06	2.1268E-06
8.57648+04	5.17728-06	5.29916-06	5.3040E-06
8.75228+04	1.1955E-05	1.22428-05	1.22548-05
8.92806+04	2.5700E-05	2.6326E-05	2.63521.05
9.1038E+04	5.1663E-05	5,29636-00	5.29954-05
9.27968+04	9.75341-05	9.99BBE - 1/5	1.00098-04
9.45548+04	1.73628-04	1.7805E-04	1.78238-04
9.63128+04	2.925DE-04	3,000BE-04	3.0039E-04
9.5070E+04	4.6804E-04	4-8037E-04	6.8087E-06
9,9828E+04	7.1378E-04	7.3285E-04	7.33636-64
1,01598+05	1,040/8-03	1.06891-03	1.07016-03
1.0334E+05	1.45536-03	1.49538-03	1.4970E-03
1.0510E+05	1.9576E-03	2.01216-03	2.01448-03
1,06866+05	2.5401E-03	2.61196-03	2.61685-03
1.0862E+05	3.1B85E-03	3.2797E-03	3.28356-03
1.1038E+05	3.88216.03	3.99468-03	3.00031-03
1,12146+05	4.5970E-03	4.751BE-03	4.73748-03
1,13896+05	5.3077E-03	5.46531-03	5.47195-03
1,1565E+05	5.99056-03	6.17068-03	6.17816-03
1,1741E+05	6.62551.03	6.82708-03	A. 8355E-03
1,1917E+05	7.19768-03	7.41926-03	7 62858-03
1,2093E+05	7.6980E-D3	7.03764-03	7.04776-03
1.2268E+05	B. 1230E-03	B. 3787E-03	8. 3805F-03
1,24448+05	B. 4741E-03	8.7638E-03	8.75524-03
1,2620E+05	8.7564E-03	Q.0381E-03	Q.0500F-03
1.2796E+05	8.9774E-03	9.26938-03	9.2817E-03
1,2972E+05	9.1459E-03	9.44655-03	80-45026-03
1,3147E+05	9.2711E-03	9.5790E-03	0.5020E-03
1.33236+05	9.3617E-03	9.6757E-03	0 ABOOF - 03
1.3499E+05	9.4253E-03	9.74468-03	Q.7581E-03
1.3675E+05	9.4685E-03	P. 7924E-03	9.80621-03
1.38516+05	9.4966E-03	9.8247E-03	Q.8386E-03
1.40268+05	9.5140E-D3	Q.8457E-D3	0.8500F-03
1,42028+05	9.5237E-03	Q.8589F-03	Q.8732E-03
1,43785+05	9.52826-03	9.8667E-03	Q. 68116.03
1.45546+05	9.52926-03	9.87076-03	Q. AR53F -03
1.4730E+05	9.52786-03	0.67231-03	Q. 8870E-03
1.4906E+05	9.52696-03	Q. 8723F-03	Q RE72E-03
1.50816+05	9.5210E-03	Q. A7136-03	Q. RRATE OF
1.52578+05	Q.51655-03	0.84041-03	Q RR278.03
1.54336+05	Q. 5116E-03	9.86755.03	0 88285-03
1.55095+05	9.50665-03	Q 86525-03	O BROKE OF
1.57858+05	0.50130-03	Q. 84275-03	0 87826-03
1.59606+05	0.40606-03	Q. R601E-03	0 875 25-03
1.61365+05	0 40075-03	0 85748-03	0 87218 .03
1.	ACHANCE -03	arminer-no	1-01915-03

1.63128+05	9.48536-03	\$.8545E-03	9.8705E-03
1.64888+05	P.4799E-03	\$.8519E-03	9.8679E-D3
1.66661+05	9.47468-03	9.84998-03	9.8652E-03
1.68395+05	9.46928-03	9.84631-03	9.8625E-03
1,7015E+05	\$.463BE-03	9.84348-03	9 .8598E-03
1.71912+05	9.45848-03	\$.8405E-03	9.8571E-03
1.73671+05	9.45306-03	9.8377E · 03	9.85436-03
1.75438+05	9.4476E - 03	\$.8368E-D3	9.8515E-03
1.77196+05	9.4422E -03	9.83186-03	9.8487E-03
1.78948+05	9.43686-03	9.82588-03	P.8458E-03
1.8070E+05	9.43121-03	9.8256E-03	9.8427E-03
1.82466+05	9.42536-03	9.62216-03	9.83936-03
1.84226+05	9.4185E-03	9.81708-03	9.8349E-03
1,85988+05	9.4098E-03	9.81126-03	9.82866-03
1.87736+05	9.39731-03	9.8006E-03	9.8182E-03
1.89495+05	9.37758-03	9.76256-03	9.8001E-03
1.91256+05	9.34521-03	9.7513E-03	9.76896-03
1,93016+05	9.29256-03	9.6988E - 03	9.7164E-03
1.9477E+05	9.2091E-03	9.61426-03	9.63196-03
1.96526+05	\$,0628E - 01	9.4847E-03	9.5022E-03
1.98286+05	B. 9000E-03	9.2961E-03	9.31346-03
2.00048+05	8.64778-03	9.0349E-03	9.051BE-03
2.01S0E+05	8.31586-03	8.69036-03	8,70666-03
2.03566+05	7.89878-93	8.2564E-03	8.2720E-03
2-05318+05	7.39736-03	7.7341E-03	7.748BE 03
2.0707E+05	6.81946-03	7.1317E-03	7.1453E-03
2.08835+~5	6.1800E-03	6.46458-03	6.47691-03
2.10598 5	5.49938-03	5.7539E-03	5.7650E-03
2.1235/ 35	4.8012E-03	5,02466-03	5,03438-03
2.34' +05	4.1099E-03	4.30216-03	4.3105E-03
2.7 61=05	3,44816-03	3.61038-03	3.61748-03
2,17626+05	2.8348E-03	2.9688E-03	2.97468-03
2.1038E+05	2.28366-03	2.39216-03	2.3968E-03
2.21146+05	1-B026E-03	1.8887E-03	1.89248-03
2 2290 0+05	1.39468-03	1.46156-03	1,4645E - 03
2.24651+05	1.05781-03	1.10886-03	1.11108-03
2.26438+05	7.8681E-D4	£.2493E-04	8.2660E-D4
2.28175+05	5.74155-04	6.0210E-04	6,0333E-04
2.20031+05	4.11204-04	4-3131E-D4	4.3220E-04
2.31601+05	2.8916E-04	3.0337E+04	3.0400E-04
2 33666404	1.0075F-04	2.09616-04	2.1005E-04
2 15206+05	1.356.18-04	1.47348-04	1,42638-04
2 3404F+05	0.05278-03	0 6/1876-06	0.62351-05
2 38726+04	5 0/2 AF - 04	A 24208-05	6 25516-05
2 2020100-00	3 RL10E-05	4 D35DE-05	4.04348-05
2 x 2 2 4 F + D	5 142 RE-05	2 54838-05	2 57366-05
5 43000+00	1 63265-06	1.61028-05	20-36816.1
3 65 255 - 53	0 44148 00	0 04 0AE - 04	0.07086.04
2 / 7636 / 0	5.76415-00	A 06128-06	6.07/28-06
2 4027640	1 1604E-00	3 64 200 -00	3 65 125 -04
5 63636 6	2 3 061 00 - 00	5 35000-04	3 16665-06
2 . 3 1038 + 03	2,0000E-00	6, 19446 · 00	D 0000E-00
£.5103E+0	0.0000E+00	0.00000000000	0.00000+00
1,00000 * 0	0.00000400	0.00001.00	0.00001+00

DISCHARGE SUMMARY FOR ALL 3 ISOTOPES PEAK-RATE PEAK-TIME TOTAL(CI) TOTAL(WEIGHTED)

1SOTOPE

N 1.				
NP237	9.52928-03	1,45546+05	9.48591+02	9.4859E+D2
U233	9.8723E-03	1.4906E+05	9.8517E+02	9.8517E+02
7H229	9.8872E-03	1.49068+05	9.86741+02	9.86741+02

TOTAL(WEIGHTED) = 2.9205E+03

AUGUT TO READ DATA SET # 2 THE INPUT ITEMS TO BE RE-READ ARE ALL OPTIONS

PARAMETERS

GROUP1 . OPTIONS

	STANDARD	PRINT, NONZERO => PRINT
OPT	ION VALUE	OUTPUT-DESCRIPTION
	1 1	LIST OF ALL PARAMETERS
	2 0	THE NETWORK LEG PROPERTIES ARRAY
114	5 B	THE NETWORK JUNCTION PROPERTIES ARRAY
	4 0	THE MIGRATION PATH PROPERTIES ARRAY
- 1	5 0	THE DECAY CHAIN PROPERTIES ARRAY
	6 0	THE ELEMENT PROPERTIES ARRAY
	7 1	FLUID VELOCITIES & SOURCE/DISCH FLOWRATES
	8 1	SUBCHAINS- DECAY, PRODUCTION, & VELOCITIES
1	9 1	SPACE & TIME STEPS AND SOURCE TYPE
1	0 1	TIME DEPENDENT OUTPUT
		. IF +N, DISCHARGE RATES EVERY NTH TIME STEP
		+ IF +N, CONCENTRATIONS EVERY NTH TIME STEP
. 1	1 1	DISCHARGE SUMMARY

EXTERNAL FILES, NONZERO => FILE WRITTEN/READ DPTION VALUE CORRESPONDING FILE

12	0	WRITE SRATE, DAT, SOURCE RATES (CI/y)
13	1	WRITE DRATE DAT, DISCHARGE RATES (CI/y)
14	0	NOT CURRENTLY USED
15	0	READ SAMP.DAT, SAMPLED DATA NORMALLY FOR REPEATED TRIALS
16	0	READ VFIELD.DAT, TIME-DEPENDENT VELOCITIES
17	0	READ SFLOW.DAT, TIME-DEPENDENT FLOWRATES
RUN	C. 180	15
OPTION	VALUE	DESCRIPTION

1.1.1.14	4415116	PRESERVER FLITON			
18	0	USE DVM(D) OR	ANALY	110 500	N(1)
10	0	ROUNE NETLINEY	203 000	LADUTY	UEIN

19	0	SOLVE NETWORK(0) OR INPUT VELOCITIES(1)
20	0	LEACH(0), SOLUBILITIES(1), OR BOTH(2)
21	0	FLOWTHRU(0), MIKCELL(1), OR CHOOSE(2)
22	0	CONSTANT(D) OR EXPONENTIAL(1) LIACH RATE
23	0	FORCE(1) USE OF LEG-TO-LEG TRANSFER ALGORITHM

DEBU	Q PRIN	TS, NONZERO => PRINT
NOTTON	VALUE	OUTPUT-DESCRIPTION
24	0	DVM MULTIPLIERS FOR TRANSPORT DISCHARGE, AND SOURCE
25	0	DIAGNOSTIC INFO FOR SUBROUTINE SAND
26	0	DIAGNOSTIC INFO FOR FUNCTION GIT
27	0	MATRIX/VECTOR SYSTEM TO BE SOLVED FOR FLOW
28	0	THE DATA FROM UNIT 10, SAMP.DAT
29	0	NOT CURRENTLY USED
30	0	INVENTORY AT RELEASE TIME
31	0	RESTRICTIONS PLACED ON THE TIME STEPS
32	0	LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
33	0	VELOCITIES FROM THE EXTERNAL FILE, UNIT 11
34	0	THE ATOK COUNT SUMMARY
35	0	JUNCTION PRESSURES & LEG FLOWRATES
36	0	LEG-TO-LEG TRANSFER FRACTIONS
37	0	TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN
38	0	TIME-DEPENDENT SOURCE FLOWRATES
WARN)	ING	"DENSITY OF SCURCE FLUID" NC JSED
WARN	ING	PORE VELOCITIES NOT USED, TINCE THEY ARE OBTAINED FROM NETWORK OR EXTERNAL FILE

FOR STEADY-STATE FLOW

LEG NO.	PORE VELOCITY
	11/4
13	2.3071E+00
14	2.3071E+00
10	2.4917E+03
3	7.8759E+02
4	7_875QE+02

PATH LENGTH FROM SOURCE BOUNDARY (ft) = 1.426.02+05AVERAGE FLUID VELOCITY (ft/y) = 7.401

FLOW RATE THROUGH SOURCE = 3.73.5E+02 ft**3/y FLOW RATE AT DISCHARGE = 1.4177E+09 ft**3/y

DECAY/PRODUCTION FACTORS AND VELOCITIES FOR EACH SUBCHAIN TRANSPORTED SUBCHAIN # DESCRIPTION DECAY/PRODUCTION

		(DECAY) NP23	7	9.93539E-01	
2		(DECAY) U233 NP237 >U233		9.17939E-01 6.19170E-03	
5	NP237	(DECAY) TH22 U233 >TH22 >U233 >TH22	9	1.49546E-01 3.62590E-02 1.55853E-04	

VELOCITY INFORMATION FOR EACH SUBCHAIN

	SIMPLE FER PLIT	LUTS		
#	MIN VELOCITY	MEAN VELOCITY	MAX. VELOCITY	MEAN COURANT NO.
1	8.92003E-01	1.25969E+00	1.52738E+00	8.84536E+00

2	8.920038-01	1,259698+00	1.62738E+00	8.84536E+00
3	8.920038-01	1.25969E+00	1.62738E+00	8.84536E+00
4	8.92003E-01	1.25969E+00	1.62738E+00	8.86536E+00
5	8.92003E-01	1.25969E+00	1.62738E+00	8.84536E+00
6	8.92003E-01	1.25969E+00	1.62738E+00	8.84536E+00

THE SPACE STEP------ DX = 2.84993E+03 FT TOTAL NUMBER OF GRID BLOCKS--- NTX = 51 WITH TOTAL CATCHER BLOCKS---- NEX = 0 THE TIME STEP------ DT = 2.00118E+04 Y FLUWTHRU SOURCE MODEL WITH 1 SOURCE BLOCKS

RADIONUCLIDE DISCHARGE RATE (C1/Y) NP237 U233 TH229 YEAR 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 2.0012E+04 0.0000E+00 0.0000E+0C 4.0024E+04 0.0000E+0C 0.0000E 0.0000E+00 0.0000E+00 6.0035E+04 0.0000E+00 6.0000E+00 0.0000E+00 8.0047E+04 0.0000E+00 0.1000E-06 0.0000E+00 4.2.114E-04 1.0006E+05 4.4543E-04 3.8541E-04 1.2007E+05 7.0456E-03 7.2/32E-03 7.2278E-03 1.4008E+05 9.51BOE-03 9.1472E-03 9.8332E-03 9.85691-03 9.4946E .03 9.8447E-03 1.6009E+05 9.4134E-03 9.8040E-03 1.8011E+05 9.7963E-03 2.90128+05 8.6455E-03 9.0556E-03 9.1073E-03 2,2013E+05 2.6538E-03 2.7788E-03 2.8008E-03 1.4713E-04 2.4014E+05 1.40296-04 1.48248-04 ± 6015E+05 1.5909E-06 1.6715E-06 1.68048-06 2.8016E+05 3.5028E-10 3.68796-10 3.7046E-10 3.0018E+05 0.0000E+00 0.0000E+00 0.0000E+00 3.2019E+05 0.0000E+00 0.0000E+00 0.0000E+00 3.4020E+05 0.0000E+00 0.0000E+00 0.00000 +00 3.6021E+05 0.0000E+00 0.0000E+00 0.0000E+00 3.80220+05 0.000000+00 0.0000E+00 0.0000E+00 .0024E+05 0.0000E+00 4 0.0000E+00 0.00005+00 4.20256+05 0.0000E+00 0.000000000 0.0000E+00 0.0000E+00 0.0000E+00 4.4026E+05 0.0000€+00 0.0000E+00 0.0000E+00 .6027E+05 0.00000:+00 .80288+05 0.0000E+00 0.0000E+00 0.0000E+00 5.0029E+05 0.0000E+00 0.0000E+00 0.0000E+00 5.20316+05 0.0000E+00 0.0000E+00 0.000CE+00 5.40328+05 0.0000E+00 0.0000E+00 D.0000E+00 5.6033E+05 0.000CE+00 0.0000E+00 0.0000E+00 U.0000E+00 0.0000E+00 0.0000E+00 5.8034E+05 6.0035E+05 0.0000E+00 0.0000E+G0 0.0000E+00 6.20368+05 0.0000E+00 0.00002+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 6.4038E+05 6.6039E+05 0.0000E+00 0.0000E+00 0,0000E+00 6.8040E+05 0.0000E+00 0.0000E+00 0.0000E+00 7.0041E+05 0.0000E+00 0.0000E+00 0.0000E+00 7.2042E+05 0.0000E+00 0.0000E+00 0.0000E+00 7.4044E+05 0.0000E+00 0.0000E+00 0.0000E+00

7.6045E+05	0.0000E+00	0.0000E+00	0.0000E+00	
7.80468+05	0.0000E+00	0.0000E+00	0.0000E+00	
8.0047E+05	0.0000E+00	0.0000E+00	0.0000E+00	
8.20486+05	0.0000E+00	0.0000E+00	0.0000E+00	
8.4049E+05	0.000LE+00	0.0000E+00	0.00000 + 00	
8.6051E+05	0.0000E+00	0.0000E+00	0.0000E+00	
8.80521+05	0.0000E+00	0.0000E+00	0.0000E+00	
9,00536+05	G.0000E+00	0.0000E+00	0.0000E+00	
9.20546+05	0.0000E+00	0.0000E+00	0,00000+00	
9.4055E+05	0.0000E+00	0.0000E+00	0.0000E+00	
9.60568+05	0.0000E+00	0.0000E+00	0.00005+00	
9.8058E+05	0.0000E+00	0.0000E+00	0.0000E+00	
1,0006E+06	0.0000E+00	0.0000E+00	0.0000E+00	
1.02068+06	0.0000E+00	0.0000E+00	0.00000 +00	

10. 1

I SOTOPE	DISCHARGE PEAK-RATE	SUMMARY FOR AL	L 3 INOTOPES TOTAL(CI)	TOTAL (WEIGHTED)
CHAIN 1 NP237 U233 TH229	9.5180E-03 9.8569E-03 9.8447E-03	.4008E+05 1.6009E+05 1.6009E+05	9.4812E+02 9.8471E+02 9.8349E+02	9.4812E+02 9.8471E+02 9.8349E+02

TOTAL (WEIGHTED) = 2.9163E+03

**** NORMAL TERMINATION ****

NEFTRAN 11 - PC VERSION RELEASED OCTOBER 1990

NEFTRAN III SAMPLE PROBLEM 2 FOR USER'S MANUAL (PC VERSION) EXECUTION DATE 11/12/1990 AND TIME 12:11:47

PARAMETERS

GROUP1 OPTIONS

STA	NDARD P	RINT, NONZERO => PRINT
OPTION	VALUE	OUTPUT-DESCRIPTION
1	1	LIST OF ALL PARAMETERS
2	1.1	THE NETWORK LEG PROPERTIES ARRAY
3	1	THE NETWORK JUNCTION PROPERTIES ARRAY
4	1	THE MIGRATION PATH PROPERTIES ARRAY
5	1	THE DECAY CHAIN PROPERTIES ARRAY
6	1.1	THE ELEMENT PROPERTIES ARRAY
7	1	FLUID VELOCITIES & SOURCE/DISCH FLOWRATES
8	1 1 1	SUBCHAINS- DECAY, PRODUCTION, & VELOCITIES
9		SPACE & TIME STEPS AND SOURCE TYPE
10	1	TIME DEPENDENT OUTPUT
		+ 1F +N, DISCHARGE RATES EVERY NTH TIME STEP
		- IF -N, CONCENTRATIONS EVERY WITH TIME STEP
11	1	DISCHARGE SUMMARY
EXT	ERNAL F	ILES, NONZERD #> FILE WRI. 7EN/READ
OPTION	VALUE	CORRESPONDING FILE
12	0	WRITE SPATE DAT, SCURCE RATES (CI/y)
13	1	WRITE DRATE.CAT, DISCHARGE RATES (C1/y)
14	0	NOT CURRENTLY USED
15	0	READ SAMP.DAY, SAMPLED DATA NORMALLY FOR REPEATED TRIALS
16	0	READ VFIELD.DAY, TIME-DEPENDENT VELOCITIES
17	0	READ SFAOW.DAT, TIME-DEPENDENT FLOWRATES
RUN	CONTRO	LS
OPTION	VALUE	DESCRIPTION
18	0	USE DYM(D) DR ANALYTIC SOLN(1)
19		SOLVE NETWORK(0) OR INPUT VELOCITIES(1)
20	0	LEACH(0), SOLUBILITIES(1), OR BOTH(2)
21	0	FLOWTHRU(D), MIXCELL(1), OR CHOOSE(2)
22	0	CONSTANT(D) OR EXPONENTIAL(1) LEACH RATE
23	0	FORCE(1) USE OF LEG-TO-LEG TRANSFER ALGORITHM
DEB	UG PRIN	TS, NONZERO => PRINT
OPTION	VALUE	OUTPUT-DESCRIPTION
24	0	NUN HUTTEDITEDE FOR TRAVEDORT ATCOURDER AND ENVERT

25 0 DIAGNOSTIC INFO FOR SUBROUTINE BAND

26	0	DIAGNOSTIC INFO FOR FUNCTION GIT
27	0	MATRIX/VECTOR SYSTEM TO BE SOLVED FOR FLOW
28	0	THE DATA FROM UNIT 10, . AMP.DAT
29	0	NOT CURRENTLY USED
30	0	INVENTORY AT RELEASE TIME
31	1.1	RESTRICTIONS PLACED ON THE TIME STEPS
32	0	LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
33	0	VELOCITIES FROM THE EXTERNAL FILE, UNIT 11
34	1	THE ATOM COUNT SUMMARY
35	0	JUNCTION PRESSURES & LEG FLOWRATES
36	0	LEG-TO-LEG TRANSFER FRACTIONS
37	1	TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN
38	0	TIME-DEPENDENT SOURCE FLOWRATES

GROUP2 - PROBLEM SIZES

ALLE	DESCRIP	TION				
2	NUMBER	OF NETI	WORK L	EGS		
0	NUMBER	OF NET	WORK J	UNCTIO	NS	
-2	NUMBER	OF MIG	RATION	PATH	LEGS	
1.1	NUMBER	OF DEC.	AY CHA	INS IN	PUT	
1	NUMBER	OF ELE	MENTS	INPUT		
					DECAY	0
				- 81	MOFR	1

DECAY CHAINS NUMBER INCLUSION MEMBERS INDEX 1 0

GROUPS . SOURCE/FLOW PARAMETERS

VALUE	DESCRIPTION
1.0000E+00	FRACTION OF SOURCE ACCESSED
0.0000E+00	PORE VOLUME CONTAINING SCURCE (ft**3)
0.0000E+00	PORE-/ CA FOR SCORCE REGIME (ft**2)
1,0146E+02	LEACH RATE (1/y)
0.0000E+00	DENSITY OF SOURCE FLUID (1b/ft**3)
0.00000 +00	PORE-AREA AT DISCHARGE (ft**2)

GROUP4 - TIME PARAMETERS

VALUE	DESCRIPTION
2.62801-02	TINE TO END OF SIMULATION (y)
0.0000E+00	TIME OF ONSET OF MIGRATION (y)
0.0000€+00	TIME OF ONSET OF LEACHING (Y)
0.0000E+00	TIME STEP FOR SOURCE (Y)
	TRANSFORT TIME STEPS FOR EACH CHAIN
	CHAIN# TIME STEP(v)
	1 0.000E+00

GROUPS . INCREMENT DETERMINATION

DEFAULT values utilized

Network Properties Array

L EQ # 1 2	inlet jct 1 2	outlet jct 2 3	Length (ft) 9.863E-02 9.043E-01	631A (54-56) 00+3000.0 00+3000.0	Hydraulic K (f1/4) 0.000E+(0 0.000E+00	&rine Conc. 0.000E+C0 0.000E+00			
Leg # 1 2	0 i epe (2 : 2 :	rsivity ft) 559E-02 559E-02	Nigrati Space Step (fl) 0.000E+00 0.000E+00	on ich Pro Diffusion No/Yes=0/ 0 1	perties Arrey 7 Mobile 1 Perceity 0.000E+00 2.60-6+01	1 wmobile Porosity 0.000E+00 1.400E+01	Mess Xfer Coef (1/y) 0.0000000 3.0 3000	Velocity (it/y) 4.609E+02 4.609E+02	
None A6	Ato Mas	mic Ei is in	em. Local dex Index	Decay Porent Par # 1 #	Chain Array ent fraction 2 From # 1	frictio FrcA #	n Inventory 2 (Ci)	Half-Life (Y)	Weighting Factor
solut	te 24	3.0	1 1	0 0	0.000£+00	0.000E+0	0 1.1816+00	3.0001+03	1.0006+00
Eion Indez 1	. \$oli x () 0.(ement P ability 2/9) DDDE+00	roporties Ar Leg Pot d R 1 1.000 2 2.005	r ny bit 1 menot Id Rt 36 = J0 0.00 26 = 00 3.70	sile 3 300E + 0 865 + 00				
	E.	DH STEAD EG NO. 1 2	PORE VI FORE VI ft, 4.601 4.602	ELOCITY /y 89E+02 89E+02					
	.P.	ATH LEN	STH FROM SOLA	CE BOUNSAR	Y (ft) = 9.8 (ft/y) = 4.6	425E-01 089E+02			
	*	LOW RATI	THROUGH SO	URCE * 0.0 ARGE * 0.0	000E+00 1:**3 000E+00 1:**3	/y /y			
THE	DETERM LEA H FORCI	INATION CH-PULS ALF-LIF NG NOMI **	OF THE TIME E RESTRICTIO E RESTRICTIO NAL # STEPS, * FINAL CHOI	STEP FOR S N, DT1 = 1 N, DT2 = 2 DTMAX = 1 CE, DT = 1	OURCE PROCEED .9713E-03y .62801-02y .3145E-03y .3145E-03y	S AS FOLLOW	\$1		

-

VTEPS IN FINDING TRANSPORT TINE STEP: MAXIMUM POSSIBLE DT = 3.062.6E-03y FOR NOMINAL # OF STEPS DT = 8.76000E-04y

DECAT/PRODUCTION FACTORS AND VELOCITIES FOR EACH SUBCHAIN TRANSPORTED SUBCHAIN # DESCRIPTION DECAT/PRODUCTION

1

ø

NO.

NO.

VELOCITY	INFORMATION FOR	EACH SUBCHAIN		
	MIN VELOCITY	MEAN VELOCITY	MAX. VELOCITY 7.013736+02	MEAN COURANT
	LEG 2	4.000076706		
	MIN VELOCITY 6.03964E+01	MEAN VELOCITY 1 2.30445E+02	MAX, VELOCITY 4.00493E+02	MEAN COURANT 1,64080E+00
	SPACE STEL	CLEG 1)	DX = 1,406071 NX = 7	1-02-11
8.0	F CATCHER BLOCK	S(LEG 1)	NC = 0	
	SPACE STE	Prise 20	DX = 1.23031	14 10-3
	# OF BLOCK	S(LEG 2)	NX = 8	
# 0	F CATCHER BLOCK	S(LEG 2)	NC = 0	
	TOTAL NUM	BER OF GRID BLOCKS	NTX = 15	
	WITH TOTA	L CATCHER BLOCKS	NEX = 0	1.1.1
	THE TIME FLOWTHRU	STEP	00047.8 * 10	E-04 T

2200

RADIONUCLIDE DISCHARGE RATE (C1/Y)

1

TEAK	solute
0.0000E+00	0.0000E+00
8.7603E-04	0.0000E+00
1.75208.03	0.00002+00
2.62801-03	1.88576-01
3.5040E-03	2.6177E+00
4.3800E-03	8.6107E+00
5.25601-03	1.81246+01
6.1320E-03	3.0178E+01
7.0080E-03	4.3460E+01
7.8840E-03	5.6750E+01
8.7600E-03	6.9159E+01
9.63601-03	8.0075E-01
1.05126.02	8.9317E-01
1.1388E-02	9,6787E 01
1.22646-02	1.020.1+02
1.3140£+02	1.0447E+02
1.40166.02	1.0288E+02
1.48928.02	9.71088+01
1.5768E - 02	8.7932E+01
1.66448-02	7.36405+01
1.75208+02	6,45568+01
1.8396E-02	5.2760E+01
1.92728-02	4.19895+01
2.01488-02	3.26428+01
2.10246-02	2.68548401

2.1900E-02	1.8579E+01
2.2776E-02	1.3661E+01
2.3652E-02	9.8975E+00
2.4528E-02	7.0758E+00
2.5404E-02	4.9977E+00
2.6280E-02	3.4914E+00
2.7156E-02	2.4147E+00

....

9

dell'

	ATON COUNT AT	2.7594E-02 YE	ARS	
NAME	SOURCE IN	DISCHARGED	MOBILE PHASE	IMMOBILE PHASE
solute	5.965E+21	5.943E+21	5.6048+18	1.66Cc+19
TOTAL	5.965E+21	5.943E+21	5.604E+18	1.660E+19

	DISCHARGE	SUMMARY FOR	ALL 1 ISOTOPES	
ISOTOPE	PEAK-RATE	PEAK-TIME	TOTAL(CI)	TOTAL (WEIGHTED)

CHAIN 1 solute 1.0447E+02 1.3140E-02 1.1731E+00 1.1731E+00

TOTAL(WEIGHTED) = 1.1731E+00

**** ORMAL TERMINATION ****

***** NEFTRAN 11 - PC VERSION RELEASED OCTOBER 1990 * NEFTRAN II: SAMPLE PROBLEM THREE - NEFTRAN II MANUAL (PC VERSION) * EXECUTION PATE 11/12/1990 AND TIME 12:15: 5

PARAMETERS

GROUP1 - OPTIONS

ST.	ANDARD P	RINT, NONZERO #> PRINT	
OPTION	VALUE	OUTPUT-DESCRIPTION	
1	1	LIST OF ALL PARAMETERS	
2	1	THE NETWORK LEG PROPERTIES ARRAY	
3		THE NETWORK JUNCTION PROPERTIES ARRAY	
4	1.1	THE MIGRATION PATH PROPERTIES ARRAY	
5	1	THE DECAY CHAIN PROPERTIES ARRAY	
6	1	THE ELEMENT PROPERTIES ARRAY	
7	1	FLUID VELOCITIES & SOURCE/DISCH FLOWRATES	
8	1.1	SUBCHAINS- DECAY, PRODUCTION, & VELOCITIES	
9	1.1	SPACE & TIKE STEPS AND SOURCE TYPE	
10	1	TIME DEPENDENT OUTPUT	
		- IF +N, DISCHARGE RATES EVERY WTH TIME STEP	
		IF -N, CONCENTRATIONS EVERY NTH TIME STEP	
11	1	DISCHARGE SUMMARY	
EX	TERNAL F	ILES, NONZERO => FILE WRITTEN 'EAD	
OFTION.	VALUE	CORRESPONDING FILE	
12	1	WRITE SRATE.DAT, SOURCE RAYES (CI/y)	
13	1.1	WRITE DRATE.DAT, DISCHARGE RATES (CI/V)	

1.0	10 M 10 M 10	METIE NEWIETONI, NIDOUGERE ENTED (CILLA)
14	0	NOT CURRENTLY USED
15	0	READ SAMP.DAT, SAMPLED DATA NORMALLY FOR REPEATED TRIALS
16	1	READ VFIELD.DAT, TIME-DEPC"JENT VELOCITIES
17	0	READ SFLOW.DAT, TIME-DEPENDENT TLOWRATES

1

18	0	USE DVM(D) OR ANALYTIC JOLN(1)
19	1.1	SOLVE NETWORK(D) OR INPUT VELOCITIES(1)
20	0	LEACH(0), SOLUBILITIES(1), OR BOTH(2)
21	0	FLOWTHRU(D), MIXCELL(1), OR CHOOSE(2)
25	0	CONSTANT(D) OR EXPONENTIAL(1) LEACH RATE
23	0	FORCE(1) USE OF LEG-TO-LEG TRANSFER ALGORITHM

0 DVM MULTIPLIERS FOR TRANSPORT, DISCHARGE, AND SOURCE 24 25 D DIAGNOSTIC INFO FOR SUCCOUTINE BAND

20	0	DIAGNOSTIC INFO FOR FUNCTION UIT
27	0	MATRIX/VECTOR SYSTEM TO BE SOLVED FOR FLOW
28	0	THE DATA FROM UNIT 10, SAMP.DAT
29	0	NOT CURRENTLY USED
30	0	INVENTORY AT RELEASE TIME
31	1	RESTRICTIONS PLACED ON THE TIME STEPS
32	0	LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
33	1	VELOCITIES FROM THE EXTERNAL FILE, UNIT 11
34	1	THE ATOM COUNT SUMMARY
35	0	JUNCTION PRESSURES & LEG FLOWRATES
36	0	LEG-TO-LEG TRANSFER FRACTIONS
37	0	TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN

38 0 TIME-DEPENDENT SOURCE FLOWRATES

GROUP2 - PROBLEM SIZES

ALUE	DESCRIP	1179	DN	
2	NUMBER	OF	NETWORK LEGS	
0	NUMBER	OF	NETWORK JUNCTIONS	
2	NUMBER	OF	MIGRATION PATH LEGS	
1	NUMBER	OF	DECAY CHAINS INPUT	
3	NUMBER	OF	ELEMENTS INPUT	
			DECAY	CHAINS
			NUMBER	INCLUSION

0

MEMBERS INDEX 0

c

GROUP3 - SOURCE/FLOW PARAMETERS

3

VALUE	DESCRIPTION
1.0000E+00	FRACTION OF SOURCE ACCESSED
0.0000E+00	PORE VOLUME CONTAINING SOURCE (++ ** 3)
0.0000E+00	PORE-AREA FOR SOURCE REGIME (ft* ')
1.0000E-04	LEACH R'TE (1/y)
0.0000E+00	DENSITY OF SOURCE FLUID (1b/ft**3
0.0000E+00	PORE-AREA AT DISCHARGE (ft**2)

GRCHP4 - TIME PARAMETERS

VALUE DESCRIPTION 8.0000E+04 TIME TO END OF SIMULATION (y) 0.0000E+00 TIME OF ONSET OF MIGRATION (y)

0000E+00	TIME	OF ONSET	OF LEACH	ING (Y)	
0000E+03	TIME	STEP FOR	SOURCE (¥)		
		TRANS	PORT TIME	STEPS	FOR EACH	CHAIN
			CHAI:#	TIME	STEP(y)	
			1	1.	0005+03	

GROUPS - INCREMENT DETERMINATION

DEFAULT values utilized

Q, 1.

Metwork Properties Array

Leg	Inlet	Outlet	Length	Area	Hydraulic	Brine
#	jet	jet	(ft)	(sq-ft)	K (ft/d)	Conc.
1.	1	2	1.500E+00	0.000E+00	0.0005+00	0.000E+00
S	- 2	3	6.5608+02	0.000E+00	6.000E+00	0.000E+00

			Migrati	on Path	Propert	ties Array				
eg #	Dispersiv (fi)	ity s	pace Step (ft)	NO/YA	usion7 es=0/1	Mobile	Immobile Poresity	Mass Xfer Coef (1/y)	Velocity (ft/y)	
1	1.000E	- 05	0.000E+00		0 0	0008+00	0.000E+00	0.000E+00	0.000E+00	
5	1,000E	+02	1.500E+00	-	0 0	.000E+00	0,000E+00	0.0008+00	0.000E+00	
				223						
					becay ch	ain Array	a second second		Sec. and the second	
lane	A LOWI C	Elem.	LOCE	Parent	Parent	Fraction	Fraction	n Inventory	Half-Life	Weighting
AD	Mass CHAIN # 1	Index	Index	# 1	# 2	From # 1	From #	S (CI)	(y)	Factor
M243	243.0	1	1	0	0	0.000E+00	0.000E+0	0 6.0638+05	7.593E+03	1.0005+00
U239	239.0	2	2	1	0	1.000E+00	0,0000+0	0 1.307E+07	2.4408+04	1.000E+00
1235	235.0	3	3	2	0	1.000E+00	0.0006+0	0 7.463E+02	7.100E+03	1.000E+00

ä

0

lem. Index	Solubility (g/g)	Leg #	Hobil Rd	lmmobile Rd	
1	0.000E+00	12	1.900E+01 1.900E+01	0.000E+00 0.000E+00	
2	0.000E+00	1 2	1.900E+01 1.900E+01	0.000E+00 0.000E+00	
3	0.0005+00	1	1.900E+01	0.000E+00	

Field Index	TIME-I Time (y)	Leg Index	VELOCITIES Velocity (ft/y)	Saturation Fraction
1	50000.0	1 2	9.80000E-02 9.80000E-02	1.000E+30 1.000E+00
2	80000.0	12	1.96000E-01	1.000E+00 1.000E+00

FOR NONSTEADY-STATE FLOW

EARLIEST NONDISPERSED BREAKTHRU TIME (Y) = 6.6939E+03 OVER THE TOTAL PATH LENGTH (ft) = 6.5600E+02 AVERAGE FLUID VELOCITY ATTAINED (ft/ = 9.8000E-02

DECAY/PRODUCTION FACTORS AND VELOCITIES FOR EACH SUB. IN TRANSPORTED

BCHAIN		DESCRIPTIC	N DECAY/PRODU	ICT10N	
1		(DECAY) AM243	9.12755E	-01	
1.6		IDECAYS DUDIO	0 710026	-01	
3		AM263 >PU239	8.599878	- 02	
		(DECAY) U235	\$,99999E	-01	
5		PU239 >U235	2.800808	+ 02	
6		AM243 >PU239 >U235	1.246158	-03	
LOCITY	LEG 1	EACH SUBCHAIN			
	MIN VELOCITY	MEAN VELOCITY .	AX. VELOCITY	MEAN COURANT	NO.
1.1	5.143018-03	5.15789E-03	5.17278E-D3	2.40702E+01	
2	5.14301E-03	5,15789E-03	5.17278E-03	2.40702E+01	
3	5.14301E-03	5.15789E-03	5.17278E-03	2.40702F+01	
- 4	5.14301E-03	5,15789E-03	5.17278E-03	2.40702E+01	
5	5.14301E-03	5,15789E-03	5.17278E-03	2.40702E+01	
6	5.14301E-03	5.15789E-03	5.17278E-03	2.40702E+01	
	LEG 2				
#	MIN VELOCITY	MEAN VELOCITY	MAX, VELOCITY	MEAN COURANT	NO.
80 B.U	-4.19118E-02	5.15789E-03	5.22276E-02	3.43860E+00	
5	-4.19118E-02	5.157896-03	5.22276E-02	3.43860E+00	
3	-4.19118E-02	5.15789E-03	5.22276E-02	3.43860E+00	
4	-4.19118E-02	5.15789E-03	5.22276E-02	3.43860E+00	
5	-4.19:,8E-02	5.15789£ 03	5.22276E-02	3.43860E+00	
6	-4.19118E-02	5.15789E-03	5.22276E-02	3.43860E+00	
	SPACE STEP	CLEG 1)	DX = 2.1428	6E-01 FT	
	# OF BLOCKS	S(LEG 1)	NX = 6		
# 0	F CATCHER BLOCKS	S(LEG 1)	NC = 0		
	SPACE STEP	CLEG Z)	DX = 1.5000	OE+00 FT	
	# OF SLOCKS	S(LEG 2)	NX = 437		
# 0	F CATCHER BLOCKS	S(LEG 2)	NC = 38		
		and the second products	and the second second		

TOTAL NUR	ABER OF GRID BLOCKS	NTX	30.	481	
WITH TOTA	AL CATCHER BLOCKS	NEX	8	38	
THE TIME	STEP-	DT	5	1.00000E+03	1
FLOWTHRU	SOURCE MODEL				

RADIONUCLIDE	DISCHARGE	RATE (CI/Y)	
YEAR	AM243	PU239	U235
0.0000E+00	0.0000E+00	0.00008+00	0.0000E+00
1.0000E+03	0.0000E+00	0.0000E+00	0.0000E+00
2.0000E+03	0.0000E+00	0.0000E+00	0.0000E+00
3.0000E+03	0.0000E+00	0 . JOOE+00	0.0000E+00
4.0000E+03	0.0000E+00	U.0000E+00	0.0000E+00
5.0000E+03	0.0000E+00	0.0000E-00	0.0000E+00
6.0000E+03	0.0000E+00	0.0000E+00	0.0000E+00

7.0000E+03	D.0000E+00	0.0000E+00	D.0000E+00
8.0000E+03	0.0000E+00	0.0000E+00	0.00005+00
P.0000E+03	0.0000E+00	0.0000F+00	0.0000E+00
1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00
1.1000E+04	0.0000E+00	0.000GE+00	D. DOODE+00
1.2000E+04	0.00008+00	0.0000E+00	0.00008+00
* .000E+04	5.7839E-10	2.94638-08	2.89396-12
.4000E+04	2.0287E-08	1.0942E-06	1.1136E-10
1.5000E+04	1.95368-07	1.11928-05	1.1809E-09
1.6000E+04	1.07088-06	6.51798-05	7.1286E-09
1.7000E+04	4.1851E-06	2.70898-04	3.0710E-08
1.8000E+04	1.2740E-05	8.7704E-04	1.0305E-07
1.9000E+04	3.24438-05	2.37621-03	2.8931E-07
2.0000E+04	7.2056E-05	5.6158E-03	7.0841E-07
2.,000E+04	1.4314E-D4	1.18726-02	1.5514E-06
2.2000E+04	2.60838-04	2.3027E-02	3.1164E-06
2.3000E+04	4.4068E-04	4.1413E-02	5.80356-06
2.4000E+04	7.01348-04	7.01618-02	1.01798-05
2.5000E+04	1.0579E-03	1.1266E-01	1.6920E-05
2.6000E+04	1.52658-03	1.7308E-01	2.6901E-05
2.7000E+04	2.1170E-03	2.5557E-01	4.1102E-05
2.8000E+04	2.83668-03	3.6460E-01	6.06655-05
2.9000E+04	3.6864E-03	5.0449E-01	8.6829E-05
3.0000E+04	4.6601E-03	6.7905E-01	1.2087E-04
3.1000E+04	5.7483E-03	8.9188E-01	1.6416E-04
3.2000E+04	6.93228-03	1.1452E+00	2.1794E-04
3.3000E+04	8.1926E-03	1.4412E+00	2.83526-04
3.40008+04	9.5029E-03	1.7800E+00	3.61946-04
3.5000E+04	1.0838E-02	2,1617E+00	4.5424E-04
3.60006+04	1.21698-02	2,5845E+00	5.6117E-04
3.70008+04	1.3469E-02	3.0461E+00	6.8335E-04
3.8000E+04	1.4714E-02	3.5434E+00	8.2116E-04
3.9000E+04	1.5879E-02	4.0720E+00	9.7473E-04
4.0000E+04	1.6947E-02	4.6277E+00	1.14416-03
4.1000E+04	1.7900£-02	5.2050E+00	1.3288E-03
4.2000E+C4	1.8727E-02	5,7969E+00	1.52868-03
4.3000E+04	1.94208-02	6.4035E+00	1.7427E-03
4.4000E+04	1.9974E-02	7.0134E+00	1.9704E-03
4,5000E+04	2.03888-02	7.6232E+00	2.21086-03
4.6000E+04	2.0664E-02	8.2276E+00	2.4627E-03
4.7000E+04	2.0806E-02	8.8216E+00	2.7251E-03
4.8000E+04	2.0821E-02	9.4006E+00	2.99668-03
4.9000E+04	2.0717E-02	9,9605E+00	3.2762E-03
5.0000E+04	2.0503E-02	1.0497E+01	3.5624E-03

-

-

1 - Siglar M

DECAY/PRODUCTION FACTORS AND VELOCITIES FOR EACH SUBCHAIN TRANSPORTED SUBCHAIN # DESCRIPTION DECAY/PRODUCTION

1	(DECAY) AM243	9.12755E-01
23	(DECAY) PU239 AM243 >PU239	9-71992E-01 3.59987E-02
4 5	(DECAY) U235 PU239 >U235	9,999998-01 2,809808-02

-

Her Se

VELUCIT	INFORMATION P	DR EACH GUBCHAI	N		
	NTH UPLANTTY	HEAN DELECT			
	1 020/ 75.02	A DZ1EDE D	11 MAX. VI	COULTY /	MEAN CLUKANT NO.
	1.027476-02	0-36616011	2 1.03300	SE-02 4	.01403E*01
c a	1.029872-02 1.030/78.03	1.031582-0	2 1.03368	SE-02 4	.81403E+01
2	1.02947E-02	1.031588-0	2 1.03368	SE-02 4	.81403E+01
4	1.029478-02	1.03158E-0	2 1.03358	3E-02 4	.81403E+01
2	1.02947E-02	1.03158E-0	5 1 0.165	3E-02 4	.81403E+01
6	1.02947E-02	1.03158E-0	30	3E-02 4	.81403E+01
	LEG 2				
	MIN VELOCITY	MEAN VELOCI	TY MAX. VE	LOCITY	MEAN COURANT NO.
1	-5.62509E-02	1.03158E-0	2 7.68824	E-02 6	.87719E+00
2	-5.62509E-02	1.03158E-0	2 7.68824	E-02 6	.87719E+00
3	-5.62509E-02	1.031586-0	7.68824	E-02 6	87719E+00
4	-5.62509E-02	1.03158E-0	7 68826	F-02 6	R77105+00
5	-5.62509E-02	1.031585-0	7 68820	E-02 6	877106+00
6	-5 625006-02	1 071-05-0	2 7 6893/	5.00 6	10///17E+UU
0	-3.023072-02	11031306-0	c 1,000c4	02 0	.0//IYE+UU
	20402 011	D/1 EC 41		3 4/30/2	AL
	SPALE SIL	P(LEG 1)	DX 3	2.14286E-	01 F1
4	# OF BLOCK	S(LEG 1)	NX 3	6	
# OF	CATCHER BLOCK	S(LEG 1)	NC +	0	
	SPACE STE	P(LEG 2)	TATES DX 2	1,50000E+	00 FT
	# OF BLOCK	S(LEG 2)	NX a	437	
# 25	CATCHER BLOCK	\$(LEG 2)	NC =	38	
	TOTAL NUM	BER OF GRID BLO	CKS++ NTX =	481	
	WITH TOTA	L CATCHER BLOCK	(8 NEX =	38	
	THE TIME	STEP	ATTAL DI	1.00000F+	03 Y
	FLOW YRU	SOURCE MODE			
	LARD OF	and the states			
5 1000E+04	3 48756-02	2 01275+01 7	0/000.07		
5 200000-04	1 05/05-02	5 75/20-01 P	EATER AT		
5.20002+04	4.03405-02	6.3396E+J1 5.	20226-02		
5.3000E+04	4.23072-02	2.01892+01 9.	7563E - U3		
5.4000E+04	4.3280E-02	2.84928+01 1.	0947E-02		
5.5000E+04	4.3547E-02	3.05268+01 1.	50-396E-05		
5.6000E+04	4.3260E-02	3.2290E+01 1.	3194E-02		
5.7000E+04	4.2512E-02	3.3789E+01 1.	4237E-02		
5.8000E+04	4.1383E-02	3.5024E+01 1.	5216E-02		
5.9000E+04	3.9945E-02	3.6000E+01 1.	6125E-02		
6.0000E+04	3.8269E-02	3.6725E+01 1	69608-02		
6.1000E+04	3.64148-02	3.72135+01 1	7716E-02		
6.2000E+04	3.44395.02	3.76778+01 1	83025-02		
6.3000E+04	3 23015.02	3 753/5+01 1	80875.00		
6 60000004	3 03105-00	3 7/055-01 1	07012-02		
6 E000E+04	3.03102-02	7.74022101 1.	99028-02		
B. 5000E+04	C.8234E-02	3./100E+01 1.	AA78E-05		
5-5000E+C4	2.6189E-02	3.6645E+01 2.	0297E-02		
6.7000E+04	2.4198E-02	3.6056E+01 2.	05818-02		
6.8000E+04	2.2280E-02	3.5353E+01 2.	0795E-02		
6.9000E+04	2.0447E-02	3.45488+01 2.	09418-02		
7.0000E+04	1.8709E-02	3.3663E+01 2	10258-02		
	THE PAR OF	arabear. Ar	INFOR OF		

7.1000E+04	1.70718-02	3.2709E+01	2.1050E-02	
7.2000E+04	1.55368-02	3.1699E+01	2.1019E-02	
7.3000E+04	1.4107E-02	3.06518+01	2.0939E-02	
7.4000E+04	1.27808-02	2.9570E+01	2.0812E-02	
7.5000E+04	1.1555E-02	2.8470E+01	2.0643E-02	
7.6000E+06	1.0428E-02	2.7361E+01	2.0437E-02	
7.7000E+04	9.3935E-03	2.62468+01	2.0195E 02	
7.8000E+04	8.4487E-03	2.5138E+01	1.99248-02	
7.9000E+04	7.5869E-03	2,40398+01	1.96268-02	
8.0000E+04	6.8034E-03	2.2955E+01	1.9304E-02	
8.1000E+04	6.0929E-03	2.1892E+01	1.89616-02	

NAM2 AM243 PU239 U235 TOTAL	ATOM COUNT AT SOURCE IN 5.080E+27 4.697E+29 9.618E+29 1.437E+30	8.1500E+04 YEA DISCHARGED 1.454E+25 4.407E+28 6.873E+29 7.314E+29	NRS MOBILE PHASE 2.236E+24 2.656E+28 6.784E+29 7.05DE+29	1MMOBILE PHASE 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
---	--	--	---	---

1 SOTOPE	DISCHARGE PEAK-RATE	SUMMARY FOR AL PEAK-TIME	L 3 ISOTOPES TOTAL(CI)	TOTAL (WEIGHTE"
CHAIN 1 AM2+3 PU239 U235	4.3547E-^? 3.7534E+01 2.1050E-02	5.5000E+04 6.3000E+04 7.1000E+04	1.1277E+03 1.0395E+06 5.4640E+02	1,1277E+03 1,0395E+06 5,4640E+02
		TOTAL	(WEIGHTED)	1.0412E+06

**** NORMAL TERMINATION ****

DISTRIBUTION

(RESEARCH)

G. F. Birchard MS NL/S-260 U. S. Nuclear Regulatory Commission Washington, DC 20555

Linda Kovach MS NL/S-260 U. S. Nuclear Regulatory Commission Washington, DC 20555

Tim Margulies MS NL/S-260 U. S. Nuclear Regulatory Commission Weshington, DC 20555

T. J. McCartin MS NL/S-260 U. S. Nuclear Regulatory Commission Washington, DC 205

T. J. Nickelson MS NL/S-260 U. S. Nuclear Regulatory Commission Washington, DC 2055.

W. Ott MS NL/S-260 U. S. Nuclear Regulatory Commission Washington, DC 20555

J. D. Randall MS NL/S-260 U. S. Nuclear Regulatory Commission Washington, DC 20555

R.1. * phard MS *: * 007 U. * .clear Regulatory Commission Washington, DC 20555 Mel Silberberg MS NL/S-260 U. S. Nuclear Regulatory Commission Washington, DC 2055"

(NMGS HLW)

P. Altomare MS 4-H-3 U. S. Nuclear Regulatory Commission Weshington, DC 20555

Ronald Ballard MS 4-H-3 U. S. Nuclear Regulatory Commission Vashington, DC 20555

John Bradbury MS 4-H-3 c S. Nuclear Regulatory Committion Taskington, DC 20555

Pauline Brooks MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

K.C. Chang MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

Donald L. Chery, Jr. MS 4-4-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

R. B. Codell MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

DIST-1

Neil Colemar. NS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

Seth Coplan MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

Norman A. Eisenberg MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

D.J. Fehringer MS 4-H+3 U. S. Nuclear Regulatory Commission Washington, DC 20555

William Ford MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

P. S. Justus MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

Keith McConnell MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

Tin Mo MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555 M.S. Nataraja MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

Jim lark MS 4-1-3 U. S. Nuclear Regulicory Commission Washington, DC 20555

J.J. Peshel MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

J. Pohle MS 4-H-3 U. S. Luclear Regulatory Commission Washington, DC 20555

John Trapp MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

B.J. Youngblood MS 4-H-3 U. S. Nuclear Regulatory Commission Washington, DC 20555

A. Alonso-Santos Universidad Politecnica de Madrid J. Gutlerrez Abascal, 2 28008 Madrid, SFAIN

George Apostolakis University of California 5532 Boelter Hall Los Angeles, CA 90024

D.E. Billington Harwell Laboratory United Kingdom Atomic Energy Authority Oxfordshire OX11 ORA UNITED KINCDOM

DIST-2
U.S. Department of Energy (2) Yucca Mountain Project Office Attn: J. Boak J.R. Dyer P.O. Box 98518 Las Vegas, NV 89193-8518 R.L. Bras Ralph Parsons Laboratory Dept. of Civil Engineering Mass. Institute of Technology Cambridge, MA 02139 Mass. Institute of Technology(2) Dept. of Civil Engineering Attn: L.W. Gelhar, Rm 48-329 D. McLaughlin, Rm 48-329 Gambridge, MA 02139 Douglas Brosseau ERCE, Inc. 1717 Louisiana NE, Suite 202 Albuquerque, NM 87110 P. Carboneras-Martinez ENRESA Calle Emilio Vargas, 7 28043 Madrid, SPAIN Battelle Pacific Northwest Lab. Attn: C. Cole P.G. Doctor P. Eslinger A.M. Liebetrau A.E. Van Luik 3100 Port of Benton Sigma V Building Richland, WA 99352 Neil Cooper Rutherford House BNFL Risley Warrington WA36AS UNITED KINGDOM J. J. K. Daemen Department of Mining and Geological Engineering

University of Arizona Tucson, AZ 85721 35, Rue Saint-Honore 77305 Fontainbleau FRANCE P. Dickman U.S. Department of Energy Nevada Operations Office P.O. Box 98518 Las Vegas, NV 89193-8518 Center .or Nuclear Waste Regulatory Analyses (7) Southwest Research Institute Attn: Frank Dodge Christopher Frietas Ronald T. Green Presed K. Nair Wesley C. Patrick John Russell Budhi Sagar 6220 Culebra Rd. San Antonio, TX 78228-0510 University of Arizona (3) Department of Hydrology and Water Resources Attn: D.D. Evans Todd C. Rasmussen Shlomo P. Neuman Tueson, A2 85721 Ketherine N. Gaither Applied Research Technical Services, Inc. 4300 San Mateo NE, Suite A220 Albuquerque, NM 87110

G. de Marsily

Ecole des mines de Paris

D. Galson
Nuclear Energy Agency
Organization for Economic
Cooperation and Development
38, Boulevard Suchet
F-75016 Paris, FRANCE

DIST-3

S. Gomberg U.S. Department of Energy Regulatory Compliance Branch Office of Civilian Radioactive Waste Management 1000 Independence Avenue Washington, DC 20585

GRAM, Inc. (5) Attn: Michael T. Goodrich Gretchen C. Newman C. David Updegraff Krishan K. Wahi Tony Zimmerman 1709 Moon St., NE Albuquerque, NM 87112

A.L. Gutjahr Department of Mathematics New Mexico Institute of Mining and Technology Socorro, NM 87801

Sharif Heger Department of Chemical and Nuclear Engineering University of New Mexico Albuquerque, NM 87131

D.P. Hodgkinson INTERA-ECL Chiltern House 45 Station Road Henley-on-Thames Oxfordshire, RG9 1 AT UNITED KINGDOM

Francis A. Kulacki Office of the Dean College of Engineering Colorado State University Fort Collins, GO 80523

Clarence E. Lee Applied Physics, Inc. 53/3 Wyoming Blvd., NE, Suite 3 Albuquerque, NM 87109

A. Nies Institut ^cur Tieflagerung Theodor-Heuss-Strass 4 D-3300 Braunschweig FEDERAL REPUBLIC OF GERMANY

P. Prado-Herrero CIEMAT Centro de Investigaciones Energeticas Medioambientales y Tecnologicas Avda. Complutense, 22 28040 Madrid, SPAIN

C. Thegerstrom Nuclear Energy Agency Organization for Economic Cooperation and Development 38, Boulevard Suchet F-75016 Paris, FRANCE

B.G.J. Thompson HM Inspectorate of Prilution Romney House 43 Marsham Street London SWIP 3PY UNITED KINGDOM

Kenneth E. Torrance Sibley School of Mechanical and Aerospace Engineering Upson and Grumman Halls Cornell University Ithaca, NY 14850

S.L. Smith Woodcote Grove Ashley Road Epsom Surrey KT18 5BW UNITED KINGDOM

DIST-4

T. Vieno Technical Resea ch Center of Finland P.O. Box 169 SF-00181 Helsinki 18 FINLAND

Dr. Piet Zuidema NAGRA Parkstrasse 23 CH-5401 Baden, SWITZERLAND

-

SANDIA NATIONAL LABORATORIEJ

1513	R.	C.	Dykhuizen
3141	S.	Α.	Landenberger (S
3151	G .	L.	Esch
3223	P .	Α.	Davis
6310	T	0.	Hunter
6310a	F .	₩.	Bingham
6313	Τ.	Ε.	Blejwas
6315	L.	Ε.	Shephard
6340	₩.	D.	Weart
6342	D.	R.	Anderson
6342	Μ.	G.	Marietta
6344	Ε.	D.	Gorham
6400	D.	J .	McCloskey
6410	D.	Α.	Dahlgren
6415	J .	Ε.	Campbell
6415	С.	D.	Leigh
6416	Ε.	J.,	Bonano
6416	Μ.	S .	Y. Chu
6416	S .	Η.	Conrad
6416	D,	Ρ.	Gallegos
6416	С.	13	Harlan
6416	Μ.	W.	Kozak
6416	Ε.	R.	Lindgren
6416	J.	Τ.	McCord
6416	Ν.	Ε.	Olague (16)
6416	Ρ.	Ι.	Poh1
6416	L.	L.,	Price
6416	R.,	R.	Rao
6416	J.	Α.	Rollstin
8524	J.	Α.	Wackerly

DIST-5



NRC 1162 NECK 1162 SZG1 3307 BIBLIOGRAPHIC DATA SHEET	I REPORT NUMBER IABINATE by NRC ADD Vol Supp. Rev. MC ADDINGUM NUMBER (1 Sev.) NUREG/CR-5618		
2 TITLE AND SUBTITLE	SAND90-2089		
User's Manual for the NEFTRAN II Computer Code	3 DATE REPORT PUBUSHED		
	February 1991		
5 AUTHORIS	6 TYPE OF REPORT		
Natalie E. Olague, Dennis E. Longsine, James E. Campbell, and Christi D. Leigh	7. PERIOD COVERED Incluse Ceres		
P - ERFOR MING DRGANIZATION - NAME AND ADDRESS IN NRC. pravide Divided, Other or Regime, U.S. Reveleer Regulatory	Commission, and maring address of contractor, provide		
Sandis National Laboratories Albuquerque, NM 87185			
SPONSORING ORGANIZATION - NAME AND ADDRESS WINRE WAR Some #1 #80000" W consideration provide NRC Director, of and matting address." Division of Engineering Office of Nuclear Regulatory Research U. S. Nuclear Regulatory Commission Washington, DC 20555	Office of Region of S. Austrian Regulator, Communicat		
10. SUPPLEMENTARY NOTES	and the second		
The ABSTRACT DOCEMBER of this document describes the NEFTRAN II (NEtw Time-Dependent Velocity Fields) computer code and is intended to sufficient information to use the code. NEFTRAN II was develop mance assessment methodology for storage of high-level nuclear welded tuff. NEFTRAN II is a successor to the NEFTRAN and NWFT contains several new capabilities. These capabilities include: pore velocities directly to the transport model and bypass the 2) the ability to transport radionuclides in tme-dependent veloc ability to account for the effect of time-dependent saturation tion factor, and 4) the ability to account for time-dependent is source regime. In addition to these changes, the input to NEFT to be more convenient for the user. This document is divided if constating of 1) a description of all the models contained in to of the program and subprograms in the code, 3) a data input gut and sample problems. Although NEFTRAN II is the fourth generat is a complete description of the code and reference to past use be necessary.	work Flow and TRANsport in to provide the reader with bed as part of a perfor- waste in unsaturated, C/DVM computer codes and to 1) the ability to input network fluid flow model, botty fields, 3) the changes on the retarda- flow rates through the TRAN II has been modified into four main sections the code, 2) a description ide and 4) verification tion code, this document er's manuals should not		
Iz ALT WUNDS, JESCRIPTORS (L. 1) words or phrases that will assist researchers in locating the report, I	13 AVAILABILITY STATEMENT		
High-levil radioactive waste disposal, performance assessment, radionuclide transport, source-term model, analytical transport, distributed velocity method transport, matrix diffusion, leg transfer, mixing cell, time-vary velocity fields Unclass Unclass			
	16 PA)¢E		



UNITED STATES NUCLEAR REGULATORY COMMISSION WASHINGTON, D.C. 20555

OFFICIAL BUSINESS PENALTY FOR PRIVATE USE, \$300

SPECIAL FOURT CLASE FIVE POSTAGE & FEES PA O USNRC

0

PERMIT No. G-67

12055513+131 1 1A*1CH1=w1w41 C5 NPC-020M C1V F01A + F01L1CATIOLS SVCS TPS 2508-5 F05 F422 w45H1NGTON C 0555