

Resent 12/11/02



Department of Energy
Office of Civilian Radioactive Waste Management
Yucca Mountain Site Characterization Office
P.O. Box 364629
North Las Vegas, NV 89036-8629

QA: N/A

OCT 08 2002

OVERNIGHT MAIL

Janet R. Schlueter, Chief
High-Level Waste Branch
Division of Waste Management
Office of Nuclear Materials Safety
and Safeguards
U.S. Nuclear Regulatory Commission
Two White Flint North
Rockville, MD 20852

TRANSMITTAL OF SATURATED ZONE (SZ) DYNAMICALLY LINKED LIBRARY
SZ_CONVOLUTE 2.0

Reference: Ltr, Schlueter to Ziegler, dtd 6/28/02

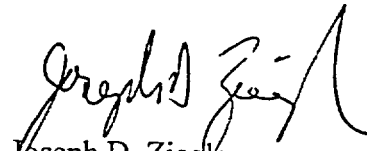
This letter transmits a CD (enclosure 1) and a hard copy directory for the CD (enclosure 2) of the *Saturated Zone Dynamically Linked Library SZ_CONVOLUTE 2.0* as requested by the referenced letter. Although no preprocessors are necessary to run the code, generic breakthrough curves are included (enclosure 3) to assist in use of the code. However, it should be noted that the executable (.exe) version of the code is not included because it is not a qualified code and was not used in the Total System Performance Assessment (TSPA)-Site Recommendation (SR) model simulations. The source code for SZ_Convolute is still being confirmed as part of the ongoing corrective action process. The source code will be provided as soon as this process is complete.

SZ_Convolute Version 2.0 .DLL is being transmitted as discussed during the August 27, 2002, telephone discussion between the U.S. Nuclear Regulatory Commission (NRC) and the U.S. Department of Energy (DOE). Based on the telephone discussion, NRC staff will only use SZ_Convolute 2.0 .DLL to condition their computer system for eventual receipt of SZ_Convolute 2.2. The DOE will provide SZ_Convolute Version 2.2 as soon as it is completely qualified. A user's manual for SZ_Convolute 2.0 .DLL is also included (enclosure 4). The file name SZConv_SR.DLL was used in the TSPA-SR to tie SZCONV.DLL specifically to the TSPA-SR model. The software file on the enclosed CD (SZCONV.DLL) was issued from the Software Configuration Management group and was tested and confirmed by this group to be the correct file used in the SR analysis.

MISSD7
WMP-11

OCT 08 2002

Due to Yucca Mountain Site Characterization Project configuration controls on software, we are providing a copy of the code and related enclosures to the NRC only. This letter makes no new regulatory commitments. Please direct any questions concerning this letter and its enclosures to Timothy C. Gunter at (702) 794-1343 or Drew H. Coleman at (702) 794-5537.



Joseph D. Ziegler

Acting Assistant Manager

Office of Licensing and Regulatory Compliance

OL&RC:TCG-1689

Enclosures:

1. CD of Saturated Zone Dynamically
Linked Library SZ_CONVOLUTE 2.0
2. Hard Copy of the CD Directory
3. CD of Generic Breakthrough Curves
4. SZ Convolute Version 2.0 User's Manual,
6/10/2000

cc w/encls:

OL&RC Library

cc w/o encls:

R. M. Latta, NRC, Las Vegas, NV
Margaret Chu, DOE/HQ (RW-1), FORS
R. R. Loux, State of Nevada, Carson City, NV
Alan Kalt, Churchill County, Fallon, NV
Irene Navis, Clark County, Las Vegas, NV
George McCorkell, Esmeralda County, Goldfield, NV
Leonard Fiorenzi, Eureka County, Eureka, NV
Michael King, Inyo County, Edmonds, WA
Andrew Remus, Inyo County, Independence, CA
Mickey Yarbrow, Lander County, Battle Mountain, NV
Lola Stark, Lincoln County, Caliente, NV
Arlo Funk, Mineral County, Hawthorne, NV
L. W. Bradshaw, Nye County, Pahrump, NV
David Chavez, Nye County, Tonopah, NV
Josie Larson, White Pine County, Ely, NV
R. I. Holden, National Congress of American Indians, Washington, DC
Allen Ambler, Nevada Indian Environmental Coalition, Fallon, NV
CMS Coordinator, BSC, Las Vegas, NV
N. H. Williams, BSC, Las Vegas, NV
R. B. Bradbury, MTS, Las Vegas, NV

cc w/o encls: (continued)

J. R. Dyer, DOE/YMSCO, Las Vegas, NV
D. G. Horton, DOE/YMSCO, Las Vegas, NV
W. J. Boyle, DOE/YMSCO, Las Vegas, NV
D. H. Coleman, DOE/YMSCO, Las Vegas, NV
T. C. Gunter, DOE/YMSCO, Las Vegas, NV
C. L. Hanlon, DOE/YMSCO, Las Vegas, NV
M. C. Tynan, DOE/YMSCO, Las Vegas, NV
J. D. Ziegler, DOE/YMSCO, Las Vegas, NV
R. N. Wells, DOE/YMSCO (RW-60), Las Vegas, NV
Records Processing Center = "6"
(ENCLS = READILY AVAILABLE)

To replace ~~the~~ Federal
Express package sent 11/8/02.
That you have been unable to
locate.

Enclosure 2

Directory DLL File Listing

- Aug 19 08:26 2002 sz_convolute_2.0_nrc_distl-listing 1st Page 1

QA: QA

1

2

3

4 MD5 (/SZ_CONVOLUTE-V2.0/sz-readme) = f8c250779fe457b3759c0c3585131cd2

5 MD5 (/SZ_CONVOLUTE-V2.0/SZCONV.DLL) = ae81beb306e92e25ddade80b6379913e

6 MD5 (/SZ_CONVOLUTE-V2.0/sz_convolute-V2.0.lst) = 5d744ccf2580efe24733d83

- 50129cc47

7 MD5 (/SZ_CONVOLUTE-V2.0/test1.exe) = 8eb4f24ed04e2160c81a360e7587a3c6

8 MD5 (/SZ_CONVOLUTE-V2.0/test1.f) = bf8ee8601145c78c64445d7a2e93348

9 Volume in drive E is 020816_1208

10 Volume Serial Number is 95DA-AC99

11

12 Directory of e:\SZ_CONVOLUTE-V2.0

13

14 08/16/2002 12:01p 815 sz_convolute-V2.0.lst

15 04/11/2000 02:36p 455,680 szconv.dll

16 11/27/2001 12:07p 360 sz-readme

17 09/25/2001 05:05a 357,376 test1.exe

18 09/25/2001 05:05a 2,446 test1.f

19 5 File(s) 816,677 bytes

20

21 Total Files Listed:

22 5 Files(s) 816,677 bytes

23 0 Dir(s) 0 bytes free

Enclosure 4

WBS: 1.2.5.4
QA QA

**Civilian Radioactive Waste Management System
Management & Operating Contractor**

SZ_CONVOLUTE VERSION 2.0

USER'S MANUAL

10207-UM-2.0-00

LV-2000-041

June 10, 2000

Prepared for:

U.S. Department of Energy
Yucca Mountain Site Characterization Office
P.O. Box 30307
North Las Vegas, Nevada 89036-0307

Prepared by:

TRW Environmental Safety Systems Inc.
1261 Town Center Drive
Las Vegas, Nevada 89134-6352

Under Contract Number
DE-AC08-91RW00134

DISCLAIMER

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, nor any of their employees, nor any of their contractors, subcontractors or their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or any third party's use or the results of such use of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors. The view and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Civilian Radioactive Waste Management System
Management & Operating Contractor

SZ_CONVOLUTE V2.0

USER'S MANUAL

10207-UM-2.0-00

LV-2000-041

June 2000

Prepared by:

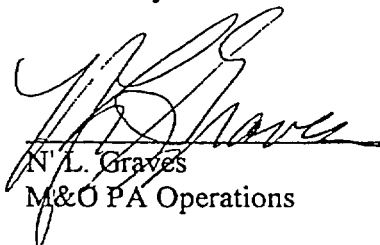


B. A. Robinson
Los Alamos National Laboratory

7/25/00

Date

Verified by:

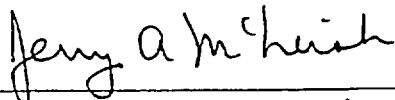


N. L. Graves
M&O PA Operations

7/25/02

Date

Approved by:

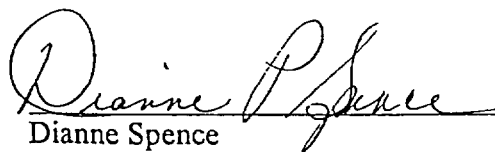


J.A. McNeish
M&O PA Operations

8.1.00

Date

ITSMA



Dianne Spence

8/3/00

Date

CHANGE HISTORY

| Revision Number | Effective Date | Description of Change |
|-----------------|----------------|--|
| 00 | 7/14/00 | Initial issue of CP1 following ITSMA review. |
| | | |

CONTENTS

| | |
|--|---|
| ACRONYMS AND ABBREVIATIONS | v |
| 1. PURPOSE AND SCOPE..... | 1 |
| 2. USER INTERACTIONS | 1 |
| 3. CONSTRAINTS AND OR SPECIAL INSTRUCTIONS. | 1 |
| 4. INPUT/OUTPUT OPTIONS | 2 |
| 5. HARDWARE AND SOFTWARE ENVIRONMENT..... | 5 |
| 6. REQUIRED TRAINING | 5 |
| 7. SAMPLE PROBLEMS..... | 5 |
| 8. INSTALLATION PROCEDURES | 6 |

ACRONYMS AND ABBREVIATIONS

| | |
|-------|---|
| CNWRA | Center for Nuclear Waste Regulatory Analyses |
| DLL | Direct Linked Library File |
| M&O | Management and Operating Contractor |
| OCRWM | Office of Civilian Radioactive Waste Management |
| PA | Performance Assessment |
| TSPA | Total System Performance Assessment |
| UM | User's Manual |
| SR | Site Recommendation |
| UZ | Unsaturated Zone |
| SZ | Saturated Zone |

1. PURPOSE AND SCOPE

This document is the User's Manual (UM) for SZ_CONVOLUTE V2.0 as required by Subsection 5.6.2 of Office of Civilian Radioactive Waste Management (OCRWM) Procedure AP-SI.1Q, Rev. 2ICN4, Software Management. SZ_CONVOLUTE V2.0 supports the Yucca Mountain Project Site Recommendation/License Application. The SZ_CONVOLUTE V2.0 code is used to evaluate radionuclide transport through the saturated zone (SZ) beneath the Yucca Mountain repository.

S. J. 8/2/00

2. USER INTERACTIONS

SZ_CONVOLUTE V2.0 is a Dynamic Link Library (DLL) that executes when called by another application. There are no direct user interactions with the software when it is operating. The user's interaction with the software consists of:

- correctly installing the software as described in the ITP,
- setting up the calling software to provide the correct inputs,
- creating a simple input text file, and
- installing generic breakthrough curve (btc) files to the proper drive and directory where they can be read by the DLL.

The user is expected to have a working knowledge of the calling application, which for the YMP, is the Total System Performance - Site Recommendation (TSPA-SR) software. Users are expected to become familiar with the software by reading the User's Manual and the other software qualification documentation as necessary. No on-line help will be provided. Should problems develop that cannot be corrected the user must contact the software developer.

3. CONSTRAINTS AND OR SPECIAL INSTRUCTIONS

The Program will require input of at least one data file containing a generic saturated-zone breakthrough curve that has been calculated for a constant mass flux input. Generic saturated-zone breakthrough curves are required for each nuclide originating at each source region and reaching each monitoring location. Any number of nuclides, source regions, and breakthrough monitoring locations can be used.

Unsaturated-zone mass flux information is required from the calling program for each nuclide at each source location.

Earlier versions of this software have been compiled without including necessary FORTRAN library files in the compilation process. These versions will only run on platforms containing the necessary library files. This problem has been recognized and corrected in this version of the software.

4. INPUT/OUTPUT OPTIONS

Input options are limited to establishing parametric values in the `sz_convolute2.dat` file. The user may also opt to create generic breakthrough curves. This process however is very complicated requiring extensive education and experience in groundwater particle transport theory and modeling along with the computer skill necessary to translate the model into a defensible computer code capable of generating the required breakthrough curves.

The program also requires input mass flux input data as a function of time. These files must be generated by the user. Examples of the mass flux input files are given in the VTP.

Inputs from the TSPA-SR software are either generated or stored in the main program or are generated by external application extensions to the main application and are passed back to the main application where they are passed on to `SZ_CONVOLUTE V2.0`. Any input or output options associated with these programs are outside the scope of this document and are not discussed.

There are no user output options other than to specify the output file name in the `sz_convolute2.dat` file.

4.1 DATA FILES

4.1.1 Output Files

An output data file, `tracks.dat`, (note, this file name may be modified in the `sz_convolute2.dat` file) will be mirror the data passed back to the TSPA-SR software. The TSPA software does not utilize this file. It is generated solely for the purpose of inspecting the results from `SZ_CONVOLUTE V2.0` for TSPA-SR realizations.

4.1.2 Input Files

As noted above generating generic breakthrough curves is beyond the scope of this document. Therefore, this discussion will be limited to creating the `sz_convolute2.dat` input file.

`sz_convolute2.dat` is a simple text file and can be created with any text editor. If a word processor is used it should be saved as a text file.

The contents of the `sz_convolute2.dat` file are described below. An example of the `sz_convolute2.dat` file is shown in Figure 1. Explanatory notes are provided in *Italics* using a smaller font

Line 1 - Alphanumeric name for the output file. This can be up to 80 characters long and may use any characters that are legal to use in a DOS file name.

Line 2 - This line contains three input data values:

- The maximum number of climate changes allowed in the analysis
- The maximum number of time steps allowed in the analysis, and
- The maximum number of saturated zone points

This data is delimited by spaces

These values are used to check for agreement between data requirements in the calling software and data provided from external files.

Line 3 - The number of radionuclide species that will be analyzed. This number must agree with the number of source term species provided by the calling software.

Line 4 - These are the flag values for each radionuclide species included in the analysis. If the value is zero they species will be skipped in the analysis. If the value is greater than zero the species will be evaluated. The value given determines which generic breakthrough curve to use. There must be 1 flag for each species and they must correspond to the correct species in the input array from the calling software. These values are delimited by spaces.

Line 5 - This value determines which column in the btc's the data will be read from.

Line 6 - This is the maximum number of climate changes that can occur in a realization. This value is used as an error check to determine whether or not the maximum number of climate changes has occurred.

Line 7 - These are the values assigned to each climate state. The values are delimited by spaces. The number of values provided should agree with the value on line 6

Line 8 - These values are concentration multipliers for each climate state, which are applied to the base case to account for flow variations between SZ and UZ. These values are delimited by spaces.

Line 9 - This value is the total time in years covered by the simulation. It is used as an error check to assure the total time is not exceeded in the analysis.

Line 10 - This value is the value of the initial time step in the TSPA-SR software

Line 11 - This value identifies the number of half life values provided for the analysis. This number should agree with the number of species given on line 3.

Line 12 - This line contains the half-life values for each radionuclide species included in the analysis. The number of values provided should agree with the value on line 11. These values are delimited by spaces.

```

tracks.dat name of the output file containing the time and associated radionuclide mass at a
           given downstream location.
           Maximum number of climate changes allowed in the analysis,
           Maximum number of time steps allowed in the analysis
5 5000 5005 Maximum number of saturated zone points

32 - number of radionuclide species to be analyzed. Must agree with the number of species in
    the calling software

species flag values - The value given determines which generic breakthrough curve to use. There
                    must be 1 flag for each species and they must correspond to the correct
                    species in the input array from the calling software
3 1 2 5 5 5 5 5 5 5 4 0 3 3 6 0 0 7 0 7 7 0 0 0 0 0 0 0 0 0 0 0

2 - breakthrough curve column to be read

3 - number of climates available

1. 2.7 3.9 - values assigned to each climate state

1.0 1.0 1.0 - concentration multiplier for the base case to account for flow variations between
             SZ and UZ

1000000.0 - total time covered by the simulation in years

125 - initial time step interval

32 - number of half lives - there must be a value for each species

half life values in years
7370.01  5.71e3  1.7e7  2.45e5  2.14e6  87.7  2.41e04  6.54e3  432.0  7.37e3
2.14e6  3.25e4  2.42e4  6.54e3  2.13e5  7.9e3  1.51e5  2.45e5  7.04e8  2.34e7
4.46e9  21.8 432.0  30.0  22.6  87.7  3.76e5  1600.0  29.1  7.54e4  68.9
1.0e12

```

Figure 1 Sample sz_convolute2.dat File

4.2 INPUT AND OUTPUT DATA DEFAULTS

There are no default values for input or output data.

4.3 FILE FORMATS

The input and output files are simple text files as discussed above.

4.4 ALLOWABLE/TOLERABLE RANGES FOR INPUTS AND OUTPUTS

In general, the input parameters in the software are not limited to specific ranges. The software should function normally with any input parameter set. However, the input parameters should be realistic.

For proper functioning of the algorithm:

- The time and breakthrough curve arrays must be monotonically increasing
- The UZ time array must be monotonically increasing
- The UZ mass flux must be ≥ 0

4.5 ANTICIPATED ERRORS AND USER RESPONSE

Three error messages are embedded within the routine. If statements perform these error checks. When a computational "divide by zero" error would occur the program branches to a write statement that writes a message (see Table 6) to the sz_convolute log file. A stop statement that interrupts the program follows the write statement.

Table 4 Program Error Messages

| .Message | Error |
|---------------------------------|--|
| Error – divide by 0, location 1 | Adjacent entries in the uz mass flux data are equivalent |
| Error – divide by 0, location 1 | The climate state multiplier for the previous climate is zero. |
| Error – divide by 0, location 1 | Adjacent entries in the uz mass flux data are equivalent |

If one of these messages occurs inspect the input data and correct as necessary.

5. HARDWARE AND SOFTWARE ENVIRONMENT.

SZ_CONVOLUTE V2.0 is a DLL application extension that will run on any PC using the Windows NT operating system with a minimum of 64 megabytes of RAM and 100 megabytes of accessible storage such as a hard drive. It is compiled as a Dynamic Link Library (DLL) file and as such can be called by any external program capable of utilizing DLL's.

6. REQUIRED TRAINING

There is no formal training for SZ_CONVOLUTE V2.0. No easily definable user skill level is applicable to this software. However, the user will need to have a working knowledge of TSPA-SR software, of SZ_CONVOLUTE V2.0, and the data passed between them. Users are expected to become familiar with the software from this Users Manual and other software qualification documentation.

7. SAMPLE PROBLEMS

Sample problems are presented in the VTP and the VTR.

8. INSTALLATION PROCEDURES

This software operates on a PC platform using the Windows NT operating system. This software operates as a DLL and must reside in the directory on the drive specified by the calling software. As a DLL (application extension) this software executes only when called by another application. This application must also be able to provide values for the input elements passed from the calling software to the routine. This application may be the TSPA-SR software or any other application capable of simulating the inputs received from the TSPA-SR software. Since this DLL cannot be independently executed proper installation and operation is established through verification testing. For this reason installation testing is limited to verifying the DLL is copied to the drive and directory specified by the calling software.

8.1 DESCRIPTION OF THE PRE-INSTALLATION TEST

No pre-installation tests are required for this software. The installer must simply verify the drives and directories specified in the main application call statement exist on the platform where the software is to be installed. If they do not exist the installer must create the directory specified by the calling software.

8.2 SOFTWARE TRANSFER TO THE TARGET PLATFORM

The software is copied to the appropriate drive and directory using the DOS copy command or the drag and drop feature in Windows.

8.3 ACTIONS NECESSARY TO COMPLETE THE INSTALLATION PROCEDURE

Install the media in the proper device capable of reading the media the software has been distributed on and copy the DLL, szconv_sr.dll, to the drive and directory specified in the calling software. The input data file, sz_convolute2.dat, and the generic breakthrough curves for each buffer zone and radionuclide species, sz_xx_yy where xx is a number identifying the buffer zone and yy is a number identifying the radionuclide species, are not distributed with the DLL. The user for their particular application must generate the sz_convolute2.dat file. The generic btc's must be generated by the user or obtained from the software developer