

Section 2

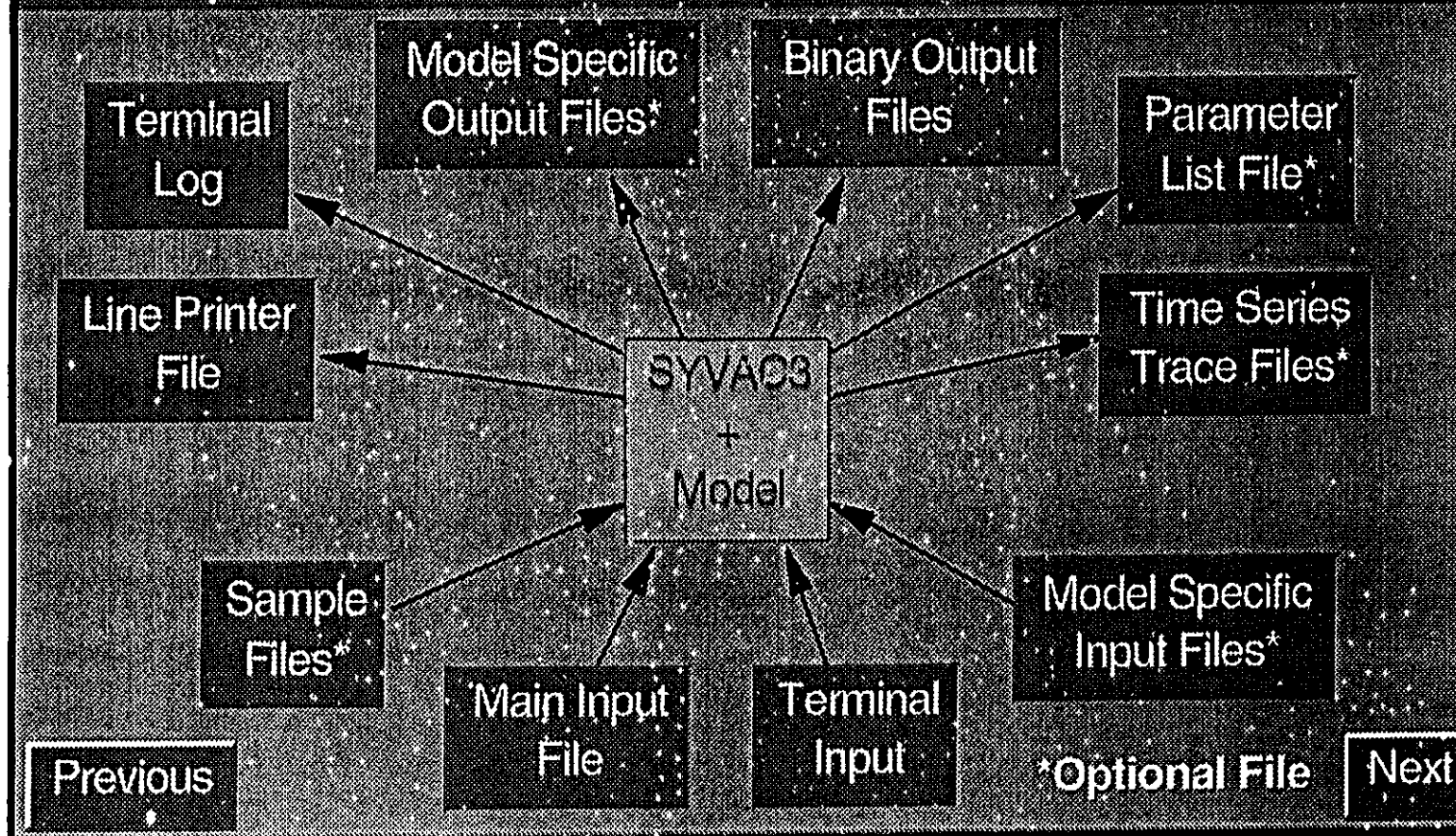
INPUT/OUTPUT

and

Systems Model Interfaces

SYVAC3: OPERATOR'S VIEW

Input and Output Files



Input Files Summary

- ◆ main input file is Svnn.INP (can be large)
- ◆ model common blocks in “.INC” files
- ◆ optional sampling files for assigning particular values, either by value or by quantile
- ◆ model defined input files
 - read using their own methods
 - read using SYVAC3 file reading (better)

SVnn.INP examples

- ◆ Section 1 - Case Control
 - descriptive title
 - define optional output files
 - numbers of simulations
 - time series controls (affect accuracy and CPU time)

Case Control Section

```
! 1997-MAY-14 VERSION 04A L. WOJCIECHOWSKI ** MEDIAN
!-----This section contains information that controls running of the case.
! Descriptive case title (ch, max 80):
! 'LEVEL E: EXACT INTERCOMPARISON MODEL'
! Output type -- 'LONG' or 'SHORT':
! 'LONG'
! Optional outputs -- a 3 ch file extension for each file required:
! 'PAR' ! 'PAR' for all parameter values
& 'SUB' ! 'SUB' for time series during submodel execution
& 'NDS' ! 'NDS' for time series containing doses from individual nuclides
& 'CDS' ! 'CDS' for time series containing doses combined from all nuclides
! Number of simulations for this case. Each range contains:
! first run number (int)
! requested number of "accepted" runs (int)
! last run number (int)
! Ranges are nonoverlapping and in increasing order:
!
! 1 1 1 ! Range 1
!& 11 1 20 ! Range 2
!& 21 1 30 ! Range 3
!
! Time series control:
!
! 1E3 1E4 1E5 1E6 1E7 2E7 ! Fixed times
! (dp ... dp, > 0, monotonically increasing)
!
! 20 250 ! Minimum and maximum number of time steps
! (int int, between 3 and MXTSTP=500)
& 0.001 ! Target fractional error for time series
! representations (dp, between 0 and 1)
& 0.10 0.10 ! Smoothing coefficients: times and values
! (dp dp, between 0 and 1)
!
```

Case Control Section (what SYVAC3 sees)

```
'LEVEL E: EXACT INTERCOMPARISON MODEL'  
'LONG'  
'PAR' 'SUB' 'NDS' 'CDS'  
  1 1 1  
1E3 1E4 1E5 1E6 1E7 2E7  
20 250 0.001 0.10 0.10
```

Control of Parameter Values

- ◆ assign particular value
- ◆ assign value from a particular quantile of a distribution
- ◆ assign value randomly chosen from a distribution

Connection to Embedded Models

- ◆ simple and straightforward connection
- ◆ SYVAC3 does not need to know variable names used by model
- ◆ set of 7 interface modules
- ◆ 5 are standard form straight from a template
- ◆ 2 drive the model calculation

SYVAC3 Modelling Tools

- ◆ time series management
- ◆ time series library of operations
- ◆ math library of solutions to transport DE for decay chains

SVnn.INP more

- ◆ Section 2 - list of Include files
 - SYVAC3 reads the model code to determine where variables are stored
 - part of the interface that links SYVAC3 with an embedded model

Svnn.INP more

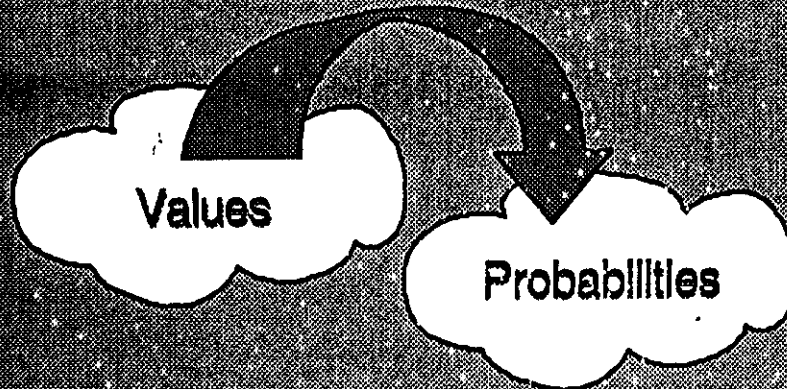
- ◆ Section 3 - Sampled Input Parameters
(grouped by sampling method)
 - variable name
 - long descriptive name
 - units
 - distribution type
 - bounds

PROBABILITY DISTRIBUTION

Definition

A random variable is a quantity which is capable of taking on various values according to chance [Kalbfleisch, 1971].

A probability distribution is an association between the set of possible values for a random variable and a set of numbers called probabilities (or probability densities).



Return

Next

PROBABILITY DISTRIBUTION

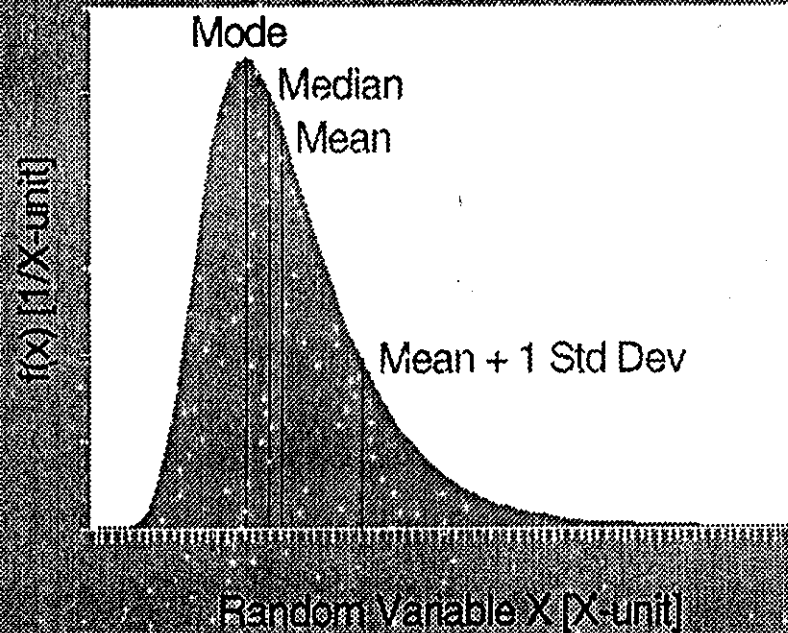
Important statistics

Mean: average value

Median: x-value where
 $\text{cdf} = 0.5$

Mode: x-value where
pdf peaks

Standard deviation:
a measure of the
distribution width

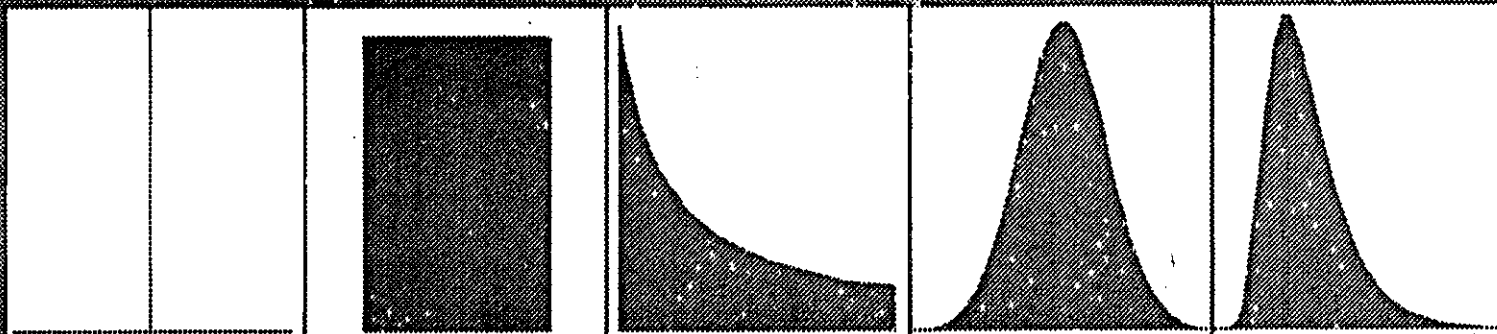


Previous

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DISTRIBUTION TYPES

Distributions Supported by SYVAC3



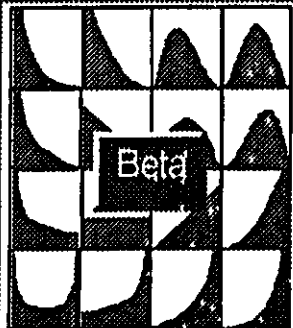
Constant

Uniform

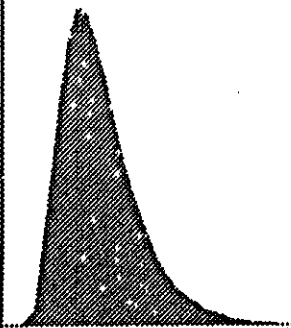
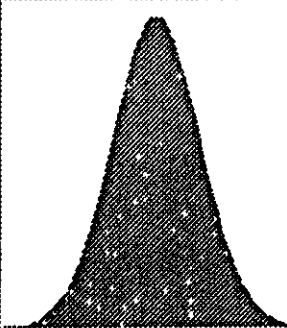
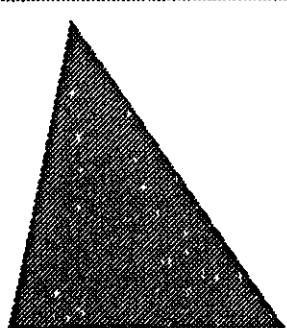
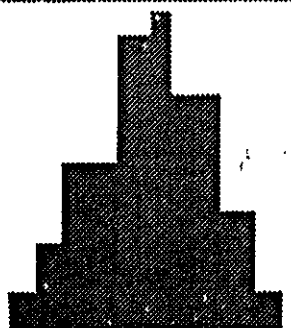
Loguniform

Normal

Lognormal



Beta



Previous

Piecewise Uniform

Triangular

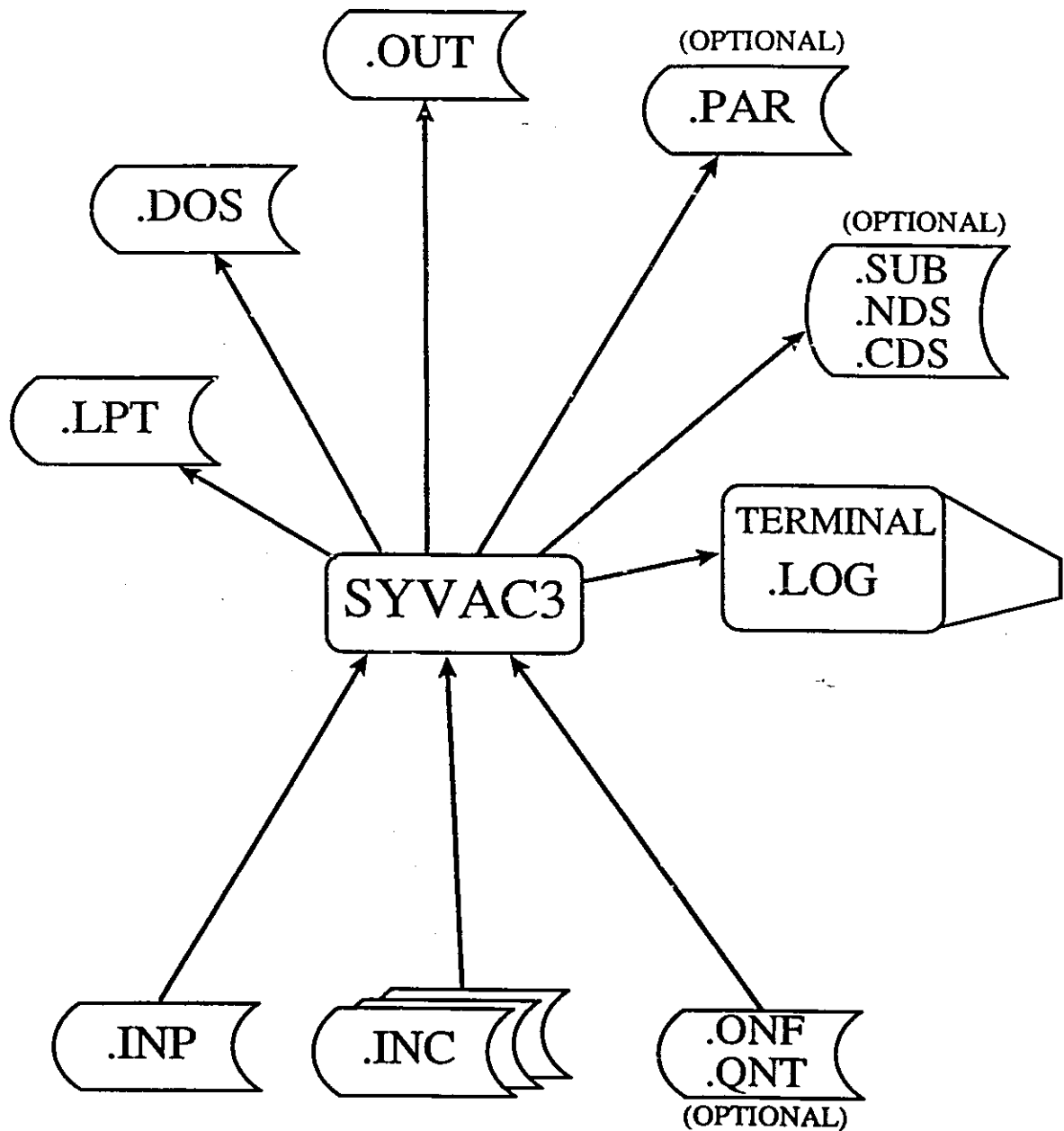
Correlated

Next

Svnn.INP final

- ◆ Section 4 - Calculated Parameters
- ◆ Section 5 - Consequence Parameters
- ◆ Section 6 - Nuclide Chains and Matrices
 - special cross reference indices are maintained to enable easy connection of chain members to data in input file

SYVAC3 OUTPUT FILES



**INFORMATION AVAILABLE
FROM
OUTPUT FILES**

- 1. Computer Usage**
(run date, CPU time, etc.)
- 2. Input Data Echo**
(parameter descriptions, pdf's, units)
- 3. Run Statistics and Error/Warning Messages**
(number of parameters, number accepted runs,
nuclide usage)
- 4. Sampled, Dependent, and Consequence
Parameter Values**
(results)
- 5. Time History of Variables**
(results)

FILE IDENTIFICATION

SV0902A1.LPT

— SVA1.INP

— LZ02

— SV309

FILE HEADERS

Filename Case Title (80 characters)	BEGUN	Date	Time
--	--------------	-------------	-------------

EXAMPLE:

SV0905U1.DOS HIGH DEMAND WELL RUNS - GROUP 1	BEGUN	14-MAY-91	08:25:15
---	--------------	------------------	-----------------

.LPT (Line PrinTer) FILE

- ASCII FILE
- ECHOES .INP FILE
- WARNING, ERROR MESSAGES
- CASE SUMMARY
- ALWAYS PRODUCED

.LPT FILE INFORMATION

- **HEADER and COPYRIGHT**
- **CASE CONTROL INFORMATION**
- **INCLUDE FILES and COMMON BLOCKS**
- **ALL PARAMETERS ARRANGED BY SAMPLING METHOD**
- **CHAINS LIST**
- **PARAMETER COUNTS**
- **WARNING and ERROR MESSAGES**
- **CASE SUMMARY**
- **CPU USAGE**

.DOS (DOSe Summary File)

- **ASCII file**
- **always produced**
- **contains case title**
- **available for use to write in (unit IUDOS) any useful information about run (eg. - summary of doses)**

.PAR (PARAmeter value) FILE

- **ASCII FILE**
- **LISTS NAMES, VALUES, AND UNITS FOR ALL SAMPLED PARAMETERS, CALCULATED CONSEQUENCE PARAMETERS**
- **OPTIONAL - CONTROLLED BY INPUT FILE**
- **USUALLY USED WITH ONLY A SMALL NUMBER OF SIMULATIONS**

.SUB (SUBmodel time series) FILE
.NDS (Nuclide DoSe time series) FILE
.CDS (Combined DoSe time series) FILE

- **CONTAIN LISTINGS OF TIME SERIES TIMES AND VALUES**
- **OPTIONAL - CONTROLLED BY STRACE CALLS IN CODE AND BY INPUT FILE**
- **EACH TIME SERIES TRANSFORMATION PRINTS ONE OR MORE TIME SERIES**

.OUT (OUTput) FILE

- **BINARY, UNFORMATTED FILE**
- **READ WITH WRKOUT PROGRAM**
- **CASE SUMMARY DATA**
- **VARIABLE & NUCLIDE DESCRIPTIONS**
- **VALUES OF ALL VARIABLES (SAMPLED PARAMETERS, CALCULATED PARAMETERS, CONSEQUENCES) FOR ALL RUNS**
- **ALWAYS PRODUCED**

WRKOUT

A POSTPROCESSING CODE THAT:

- **READS CONTENTS OF SV09...OUT FILE**
- **PERFORMS OPTIONAL ANALYSES**
- **WRITES OUTPUTS TO THE TERMINAL AND/OR A FILE**

PRESENTATION OF RESULTS

- **histogram**
- **scatterplots**
- **line plots**
- **3-dimensional plots**
- **3-dimensional figures**
- **interactive displays**

Variables to Display

Type of Display

one

- histogram
- cumulative distribution
- box & whisker

one and time

- time series plot
- box & whisker

one(+) & 2D geometry

- surface plots
- "skyscrapers"

two

- scatter plot

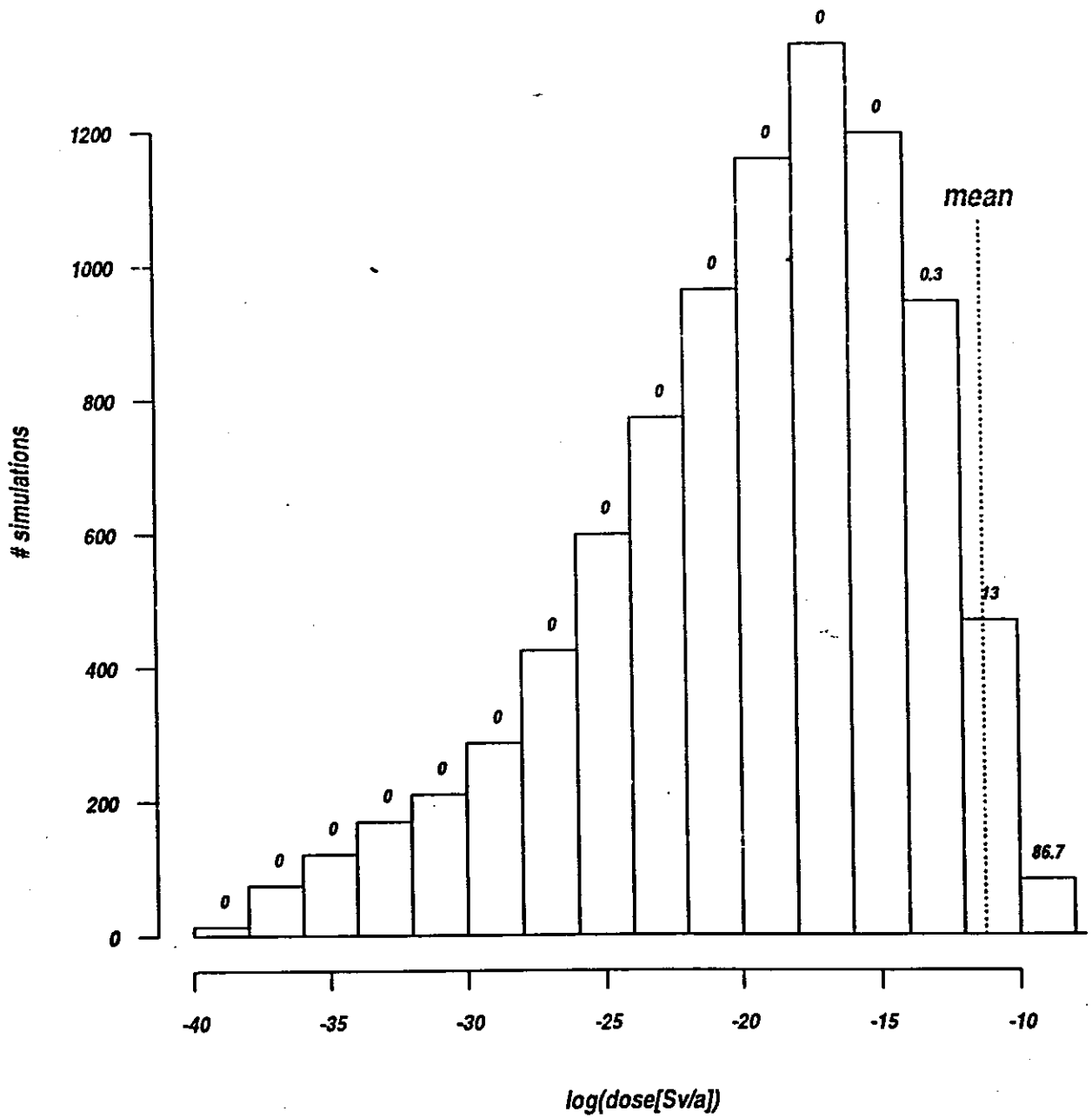
three

- labelled scatter plot
- surface plots

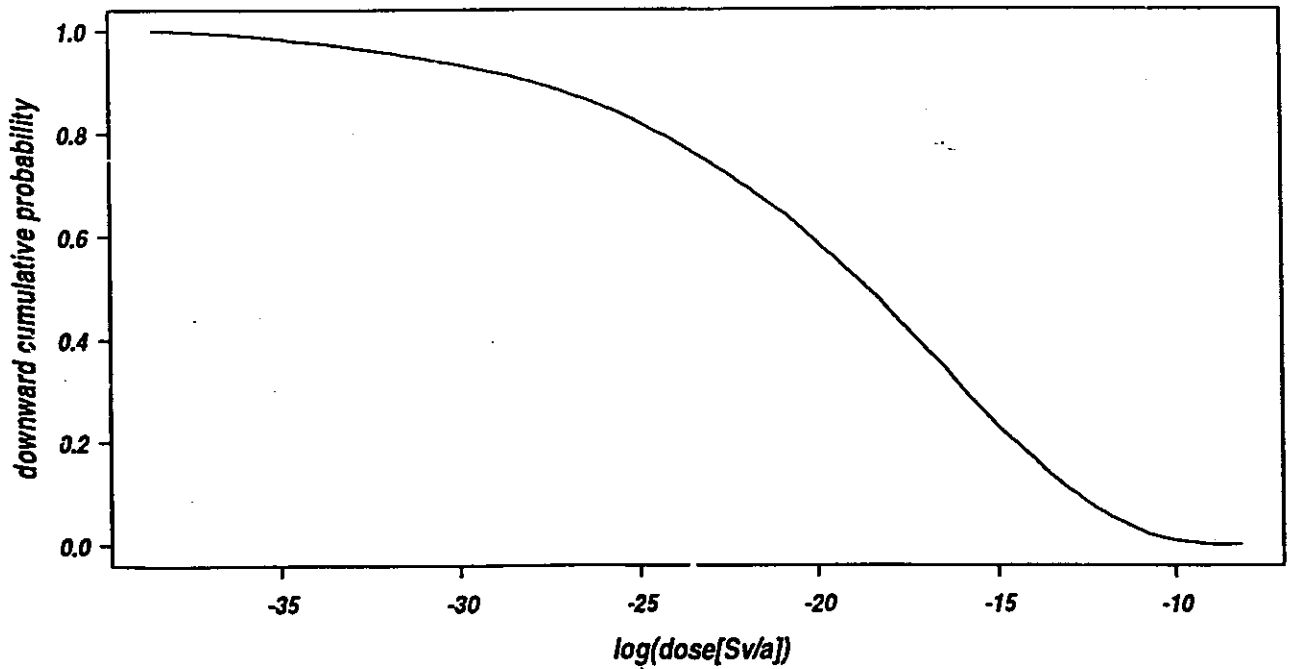
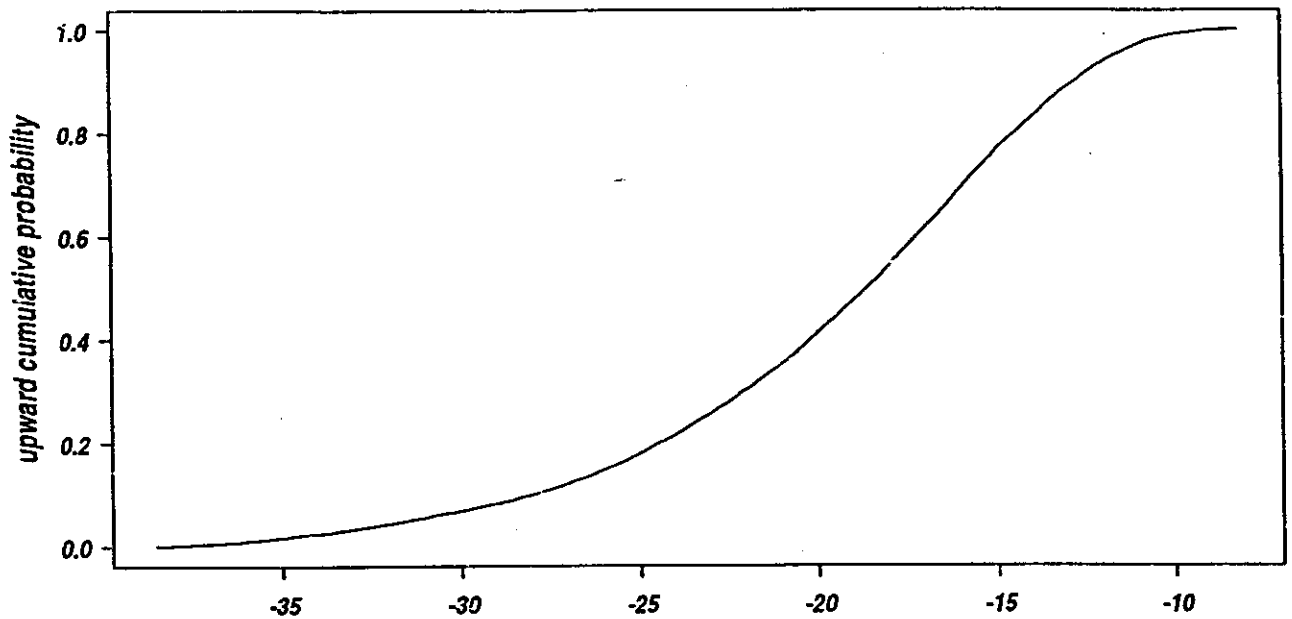
more than three

- surfaces with contours, colour

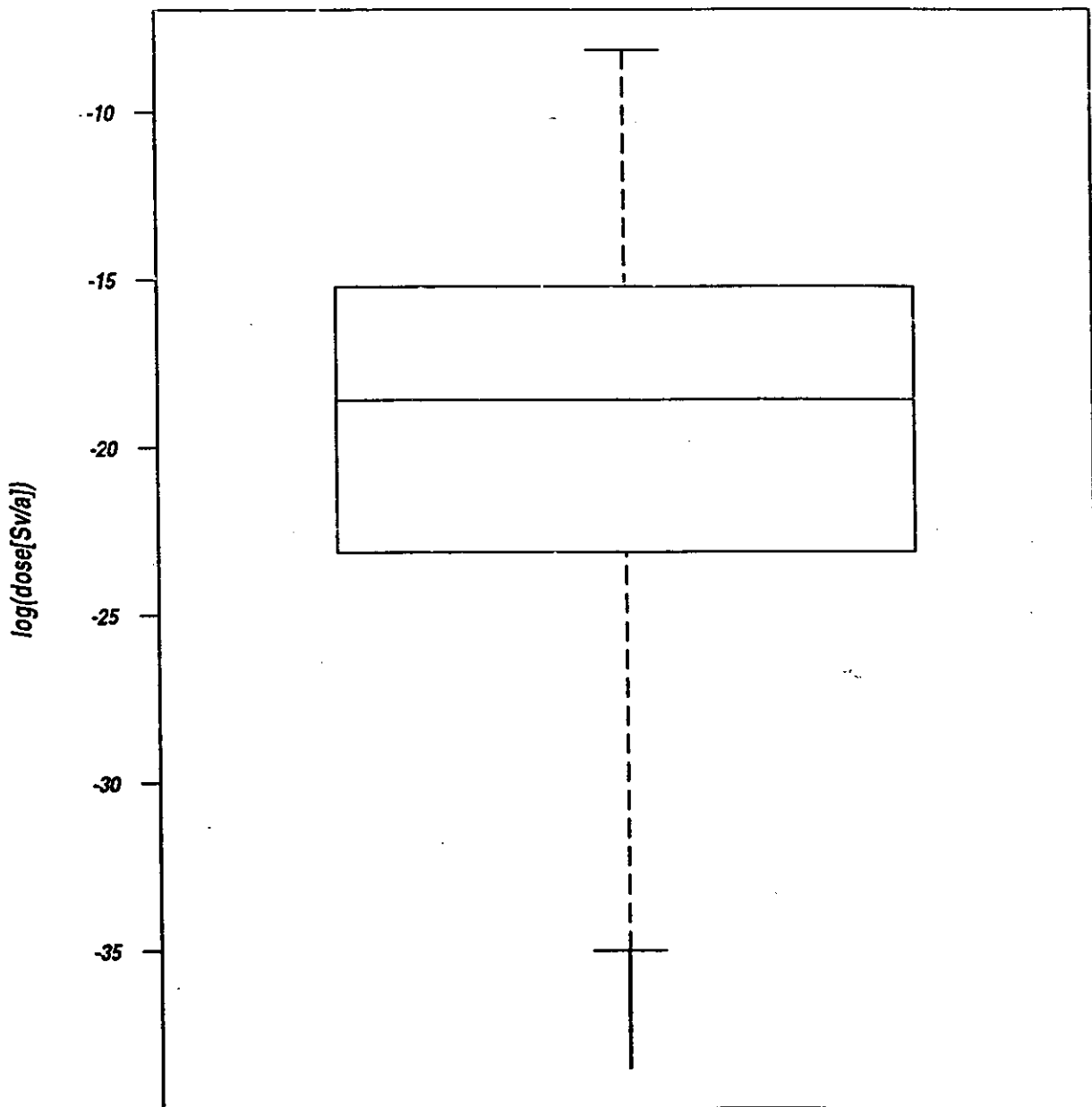
Dose from I-129 at 10,000 Years



Dose from I-129 at 10,000 Years

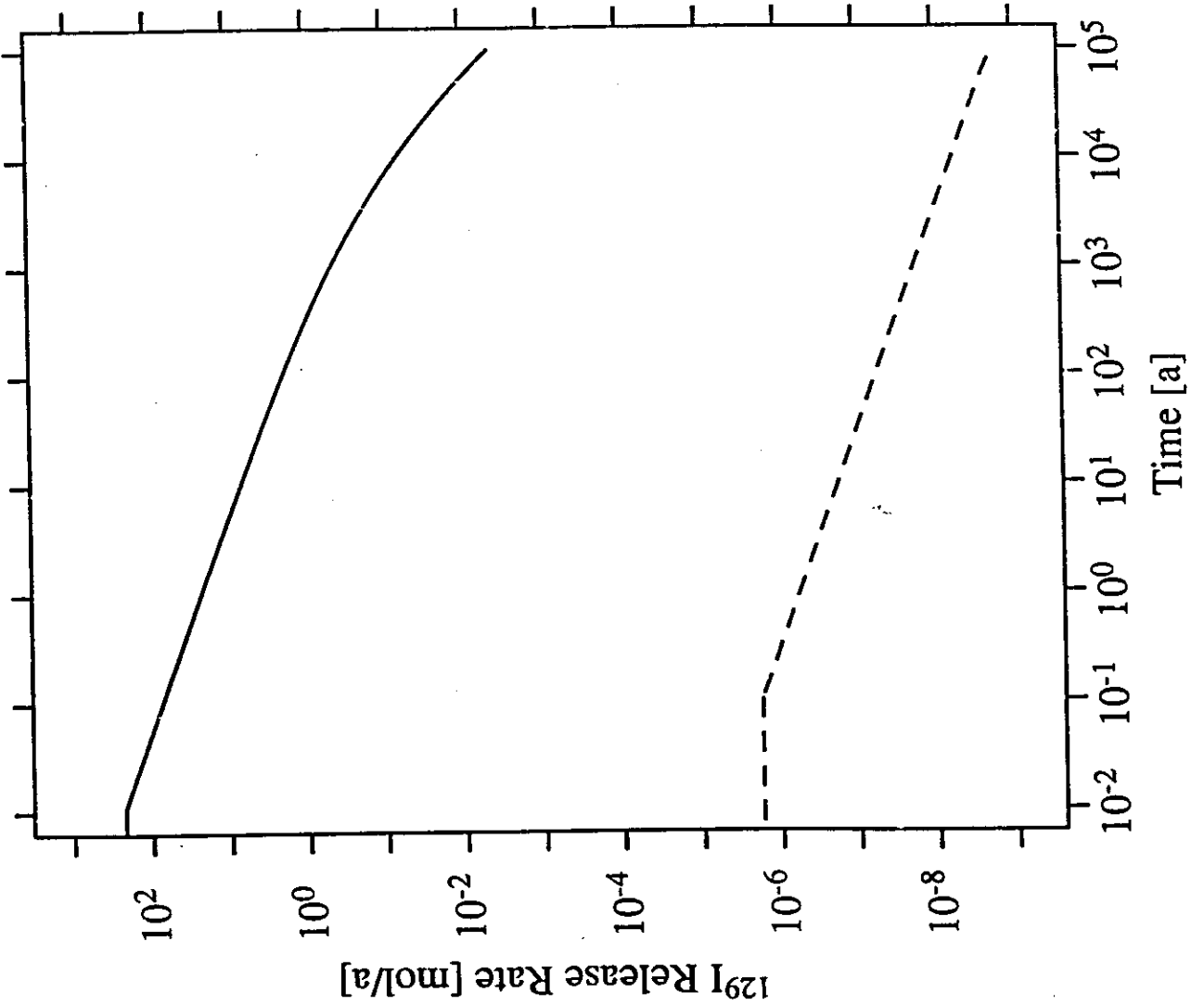


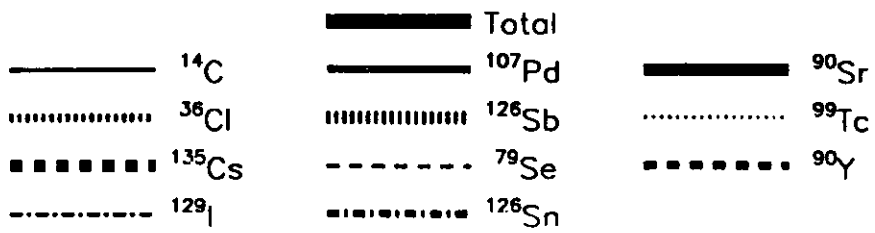
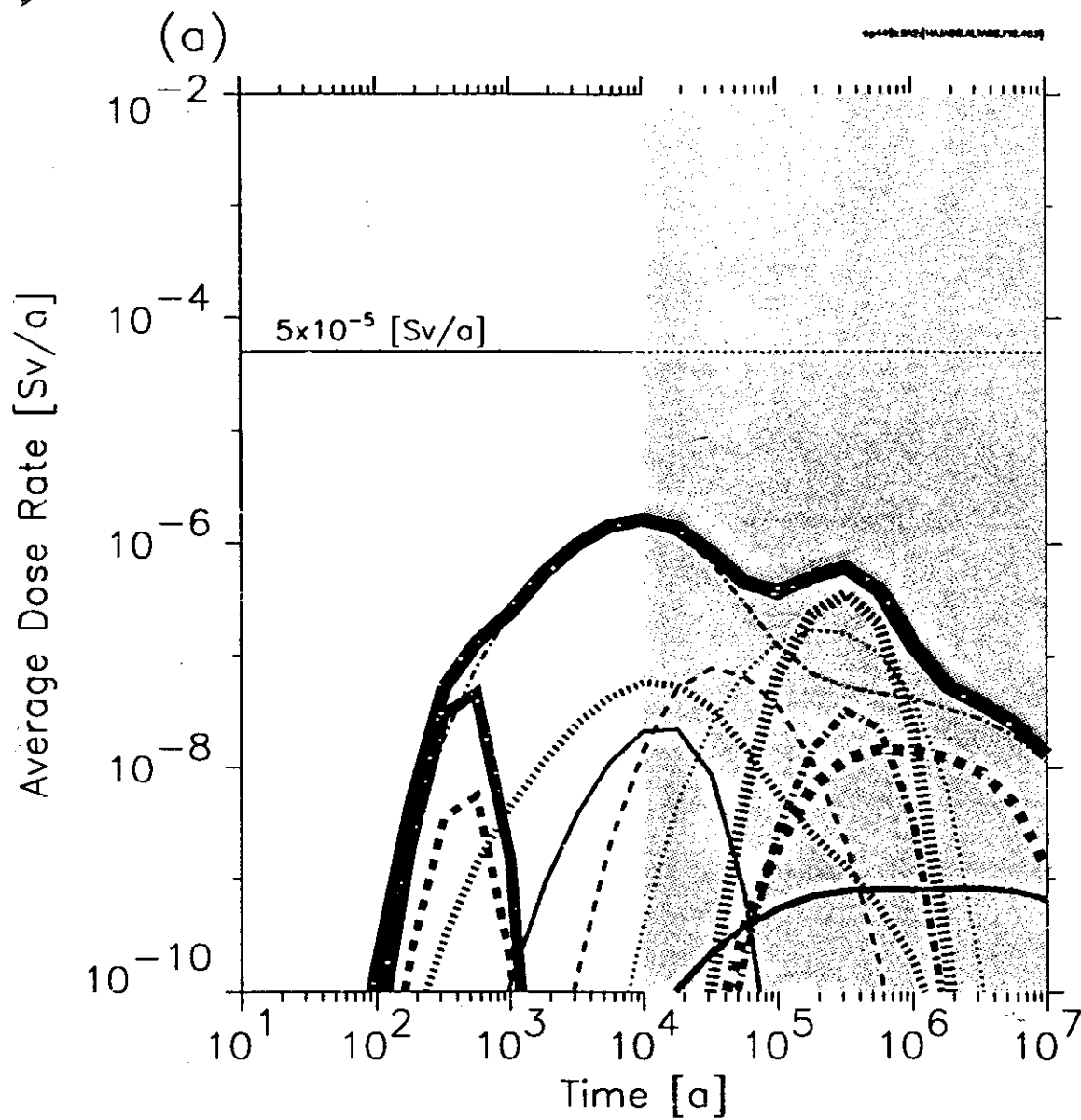
Dose from I-129 at 10,000 Years



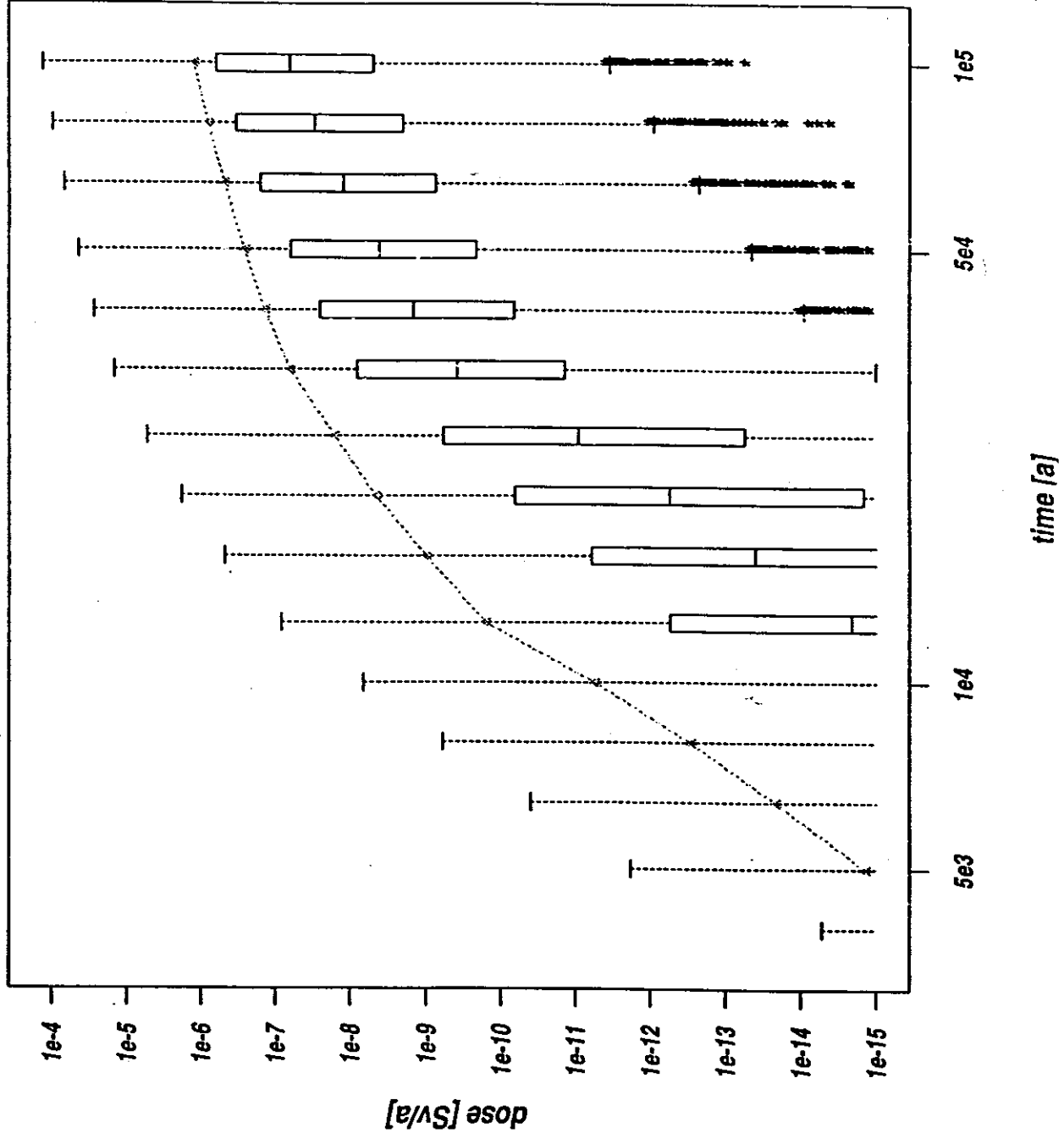
Release Rate from Wasteform

Instant Release
Congruent Release
(for Sector 1)

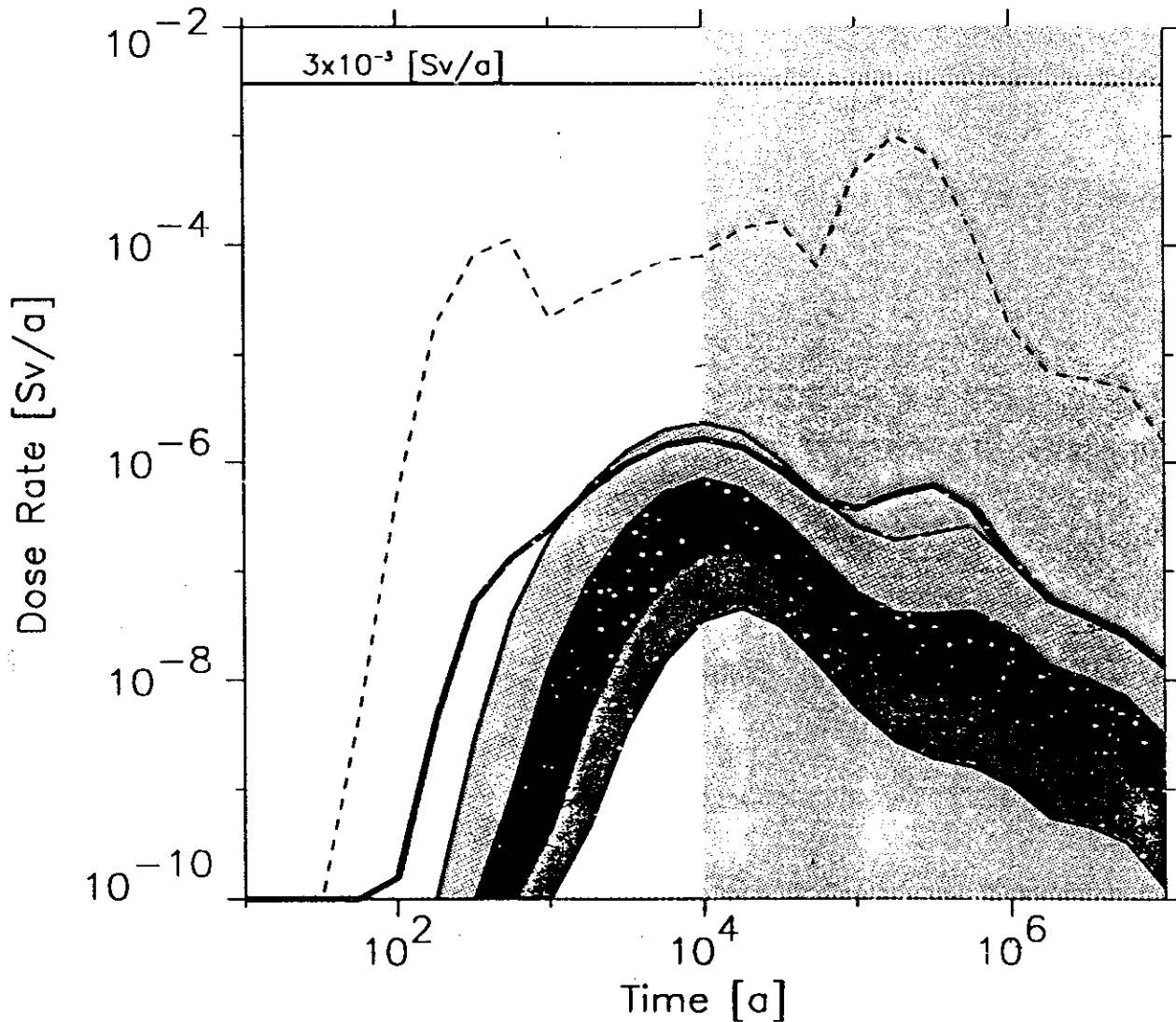




Dose from I-129

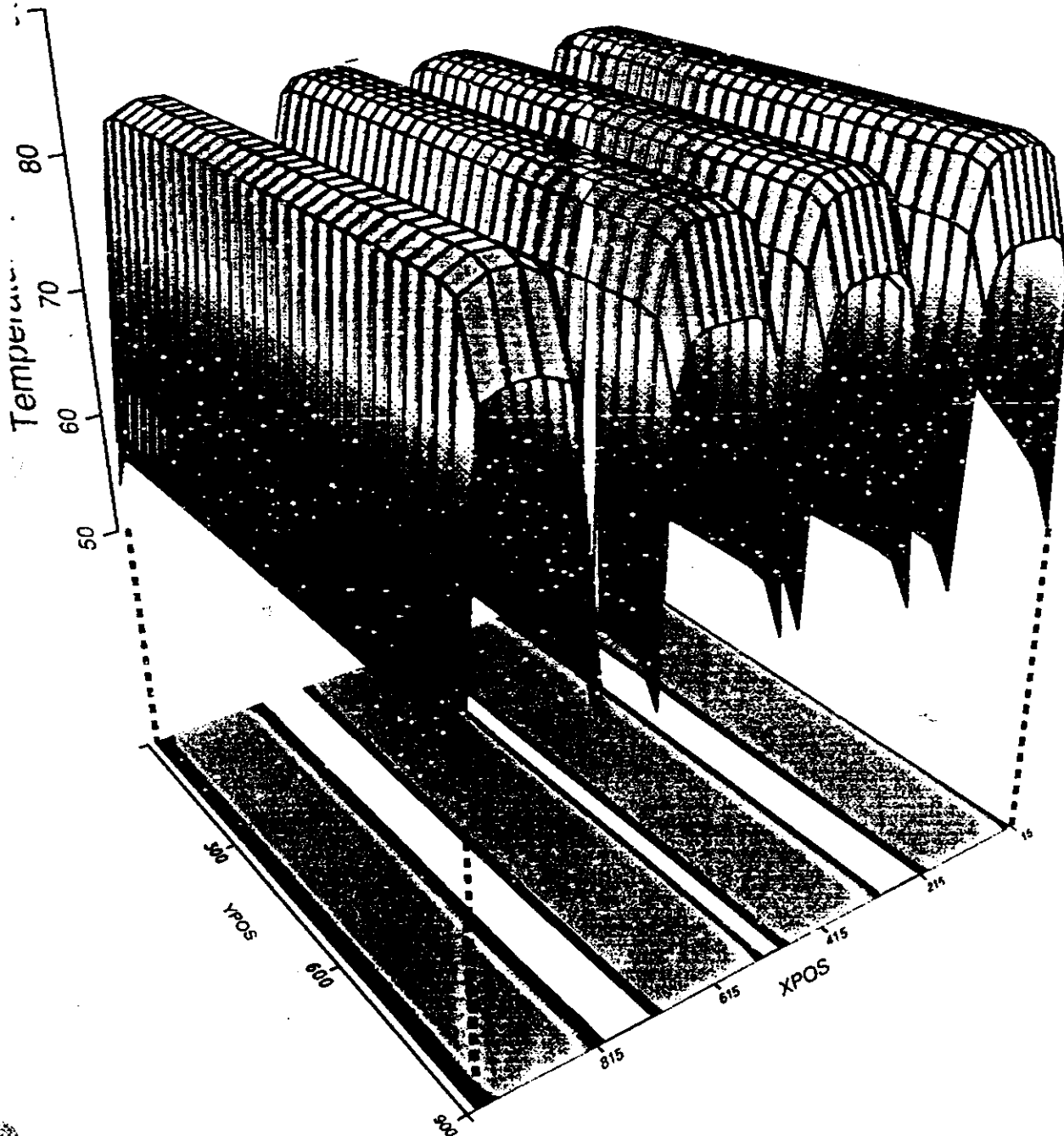


Fission Products

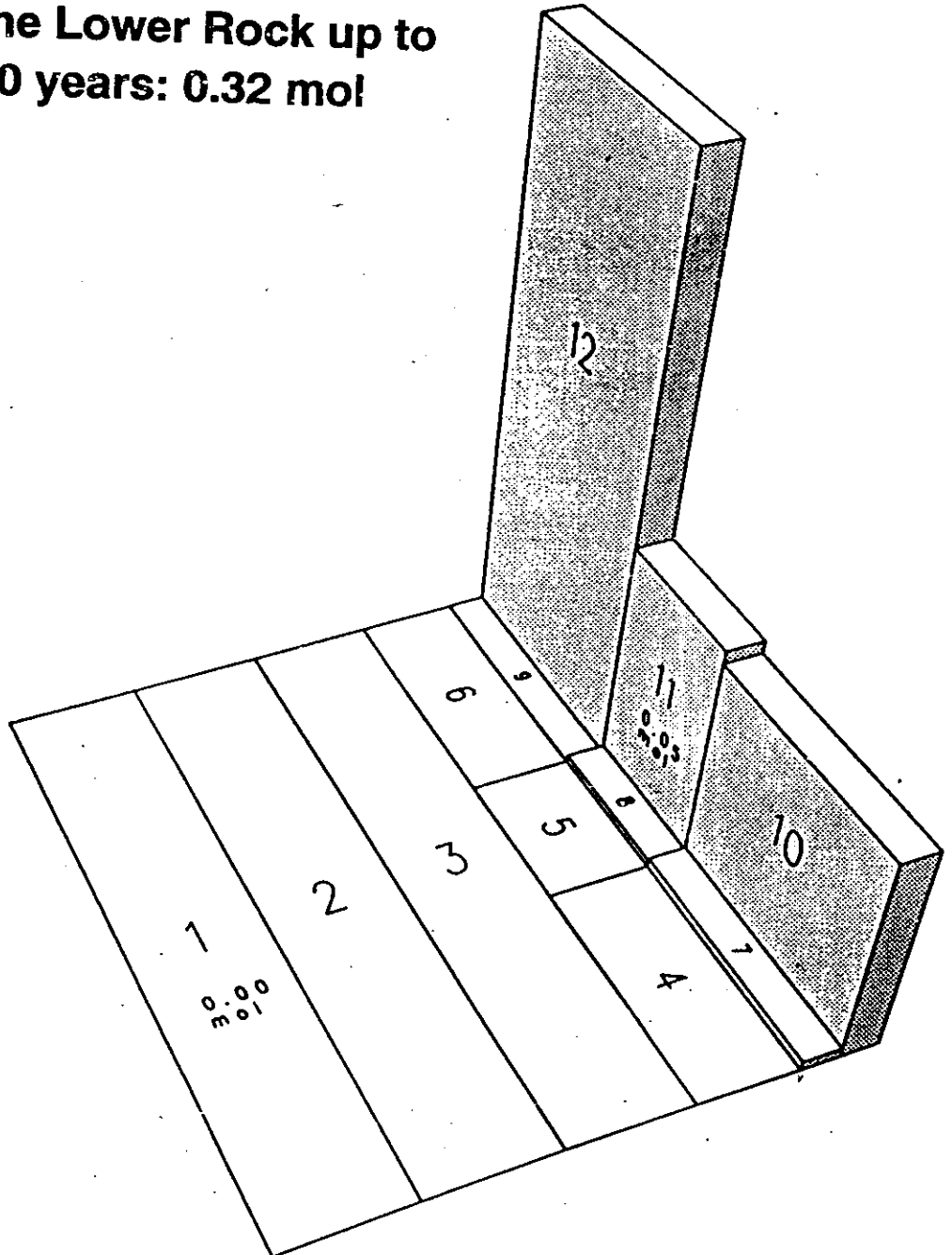


- Maximum Observed Value
- ▨ 60 to 80 Percentile
- 40 to 60 Percentile
- ▩ 20 to 40 Percentile
- Minimum Observed Value
- Average Value

Left Quadrant Temperature Profile at 10 Years

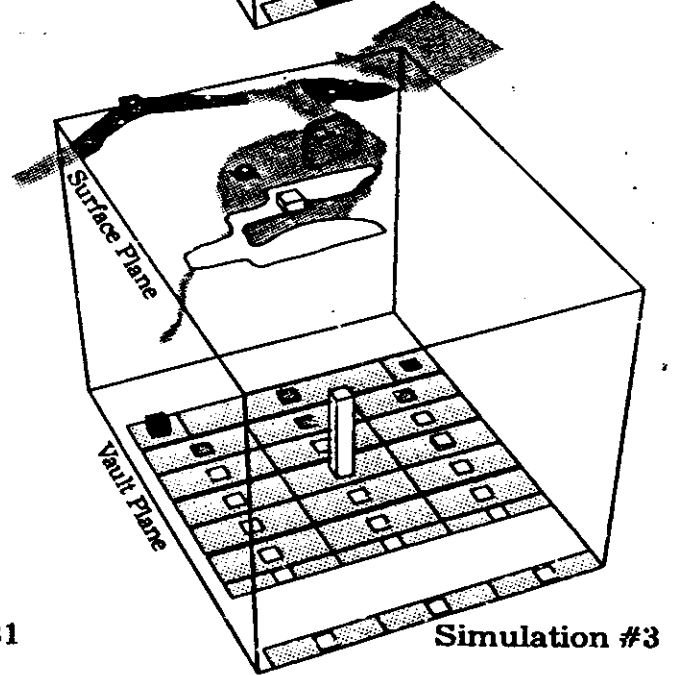
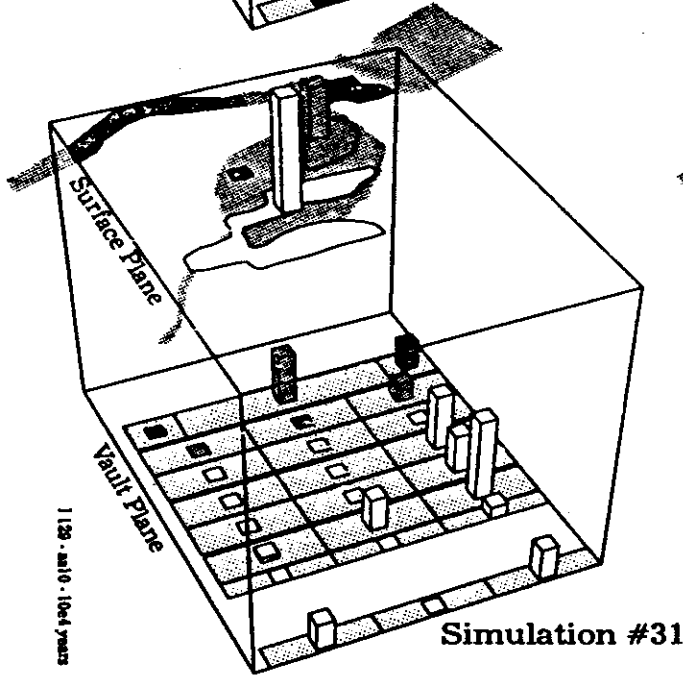
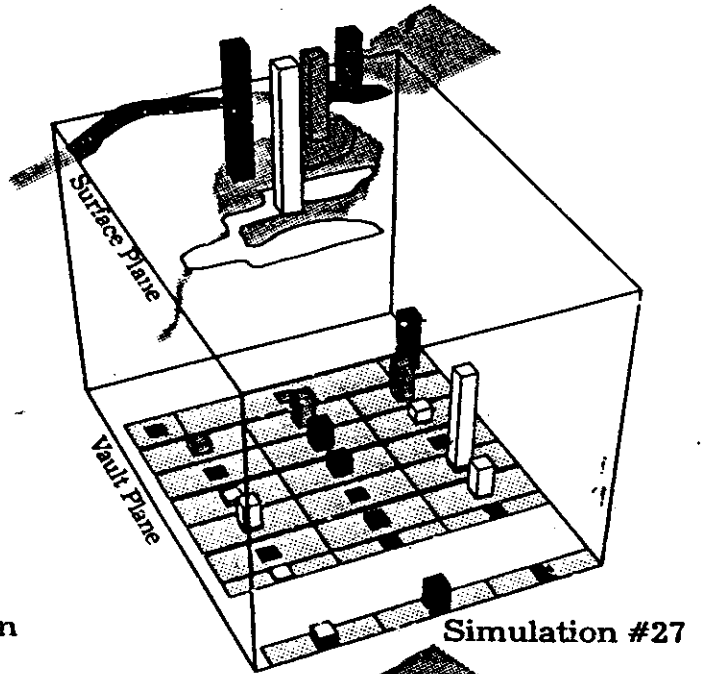
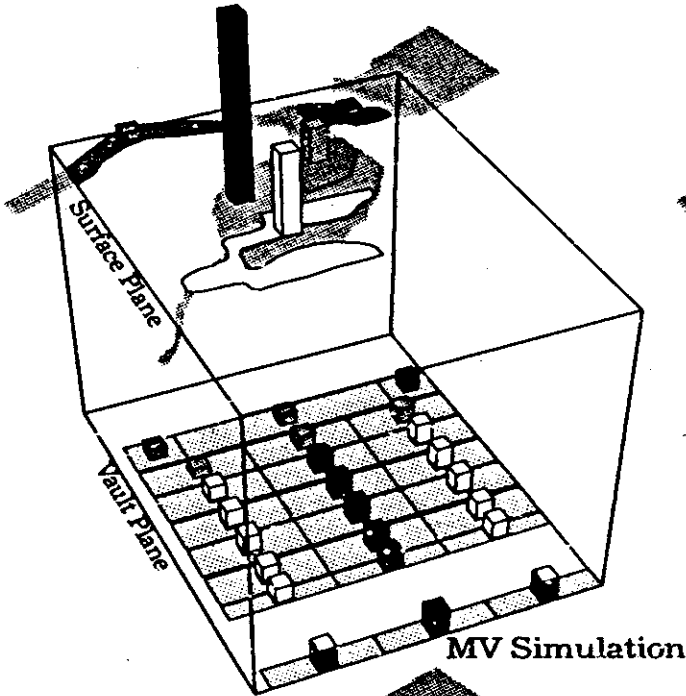


**Total Release of I_{129}
from the Lower Rock up to
100,000 years: 0.32 mol**

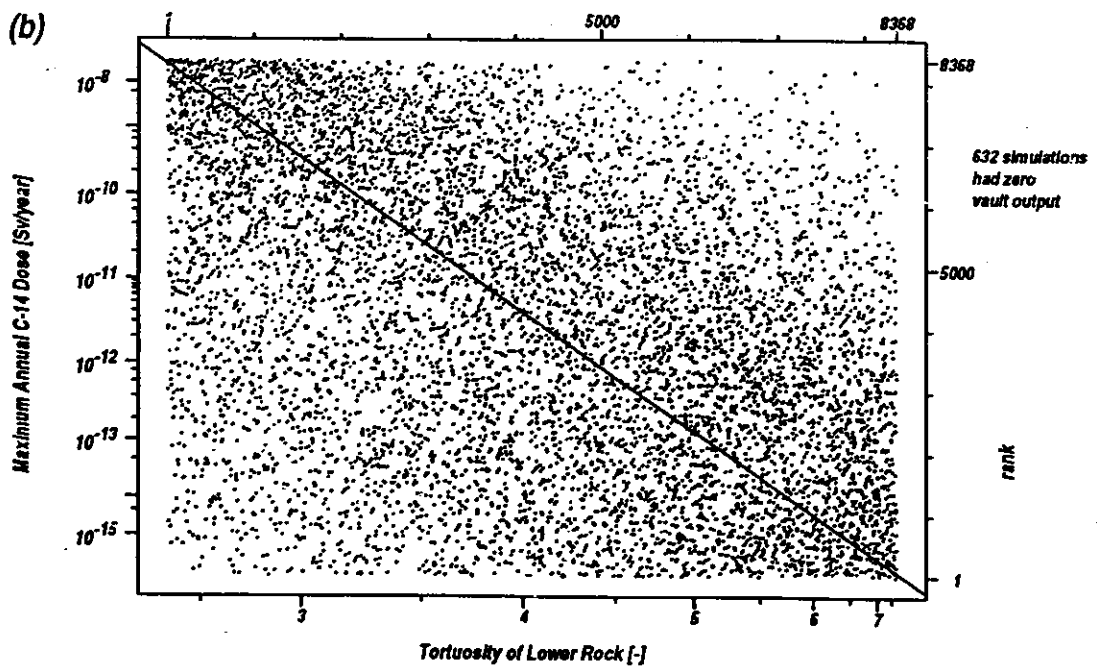
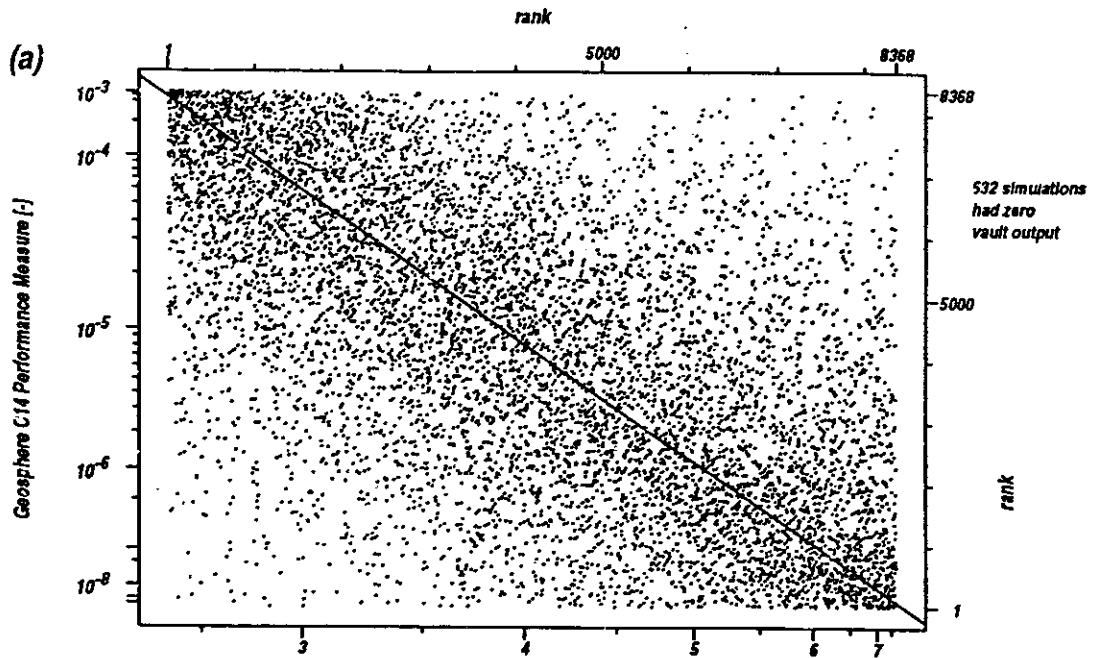


Boggy Creek North
 Pinawa Channel North
 Well

 Boggy Creek South
 Pinawa Channel South



1129 - a-10 - 1064 years



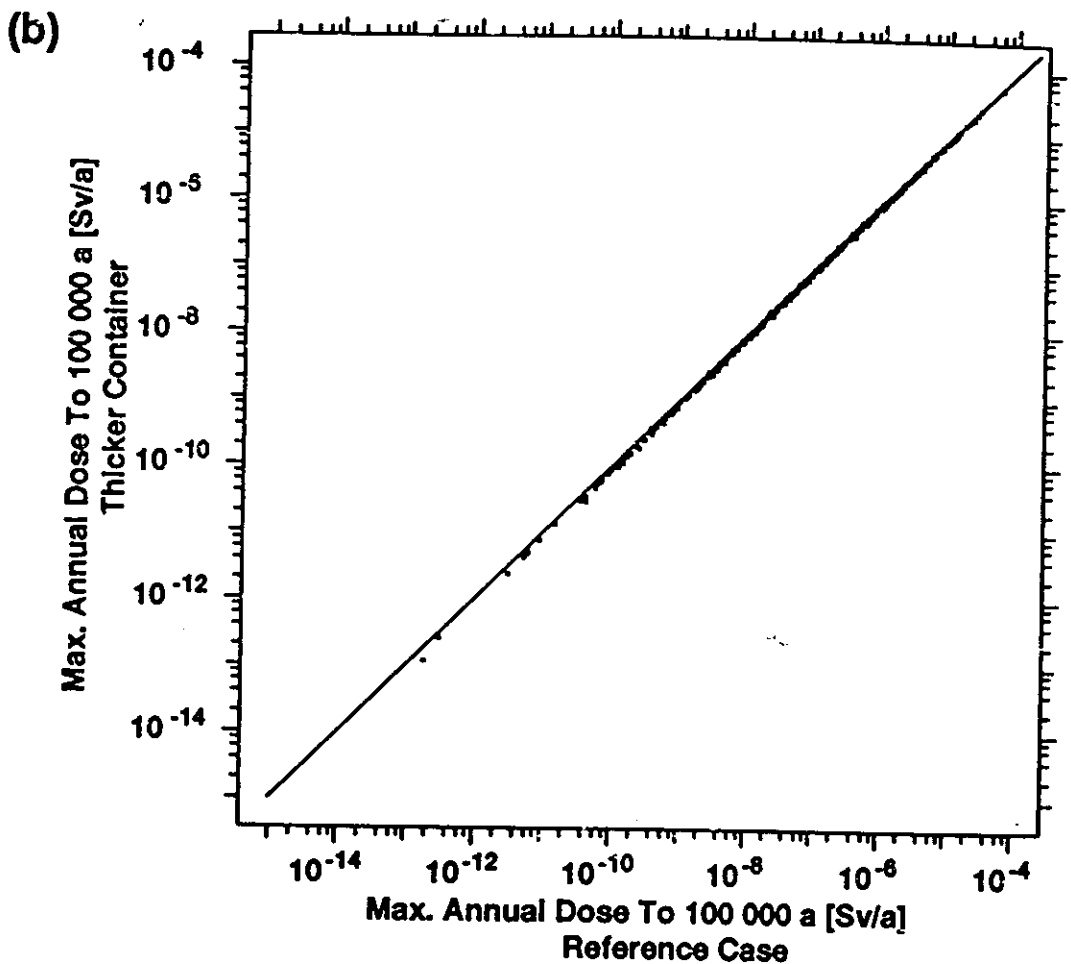
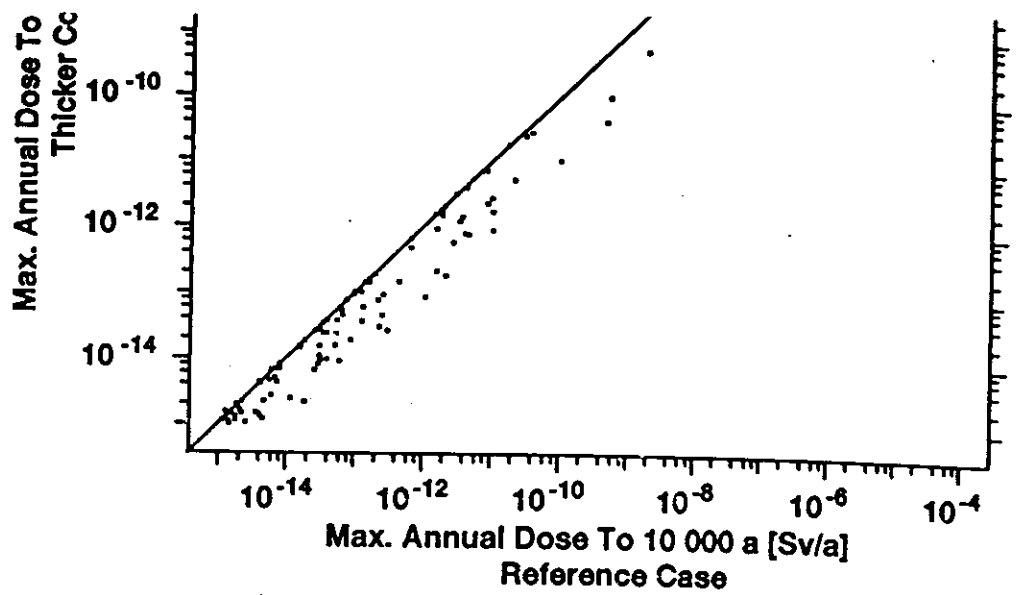
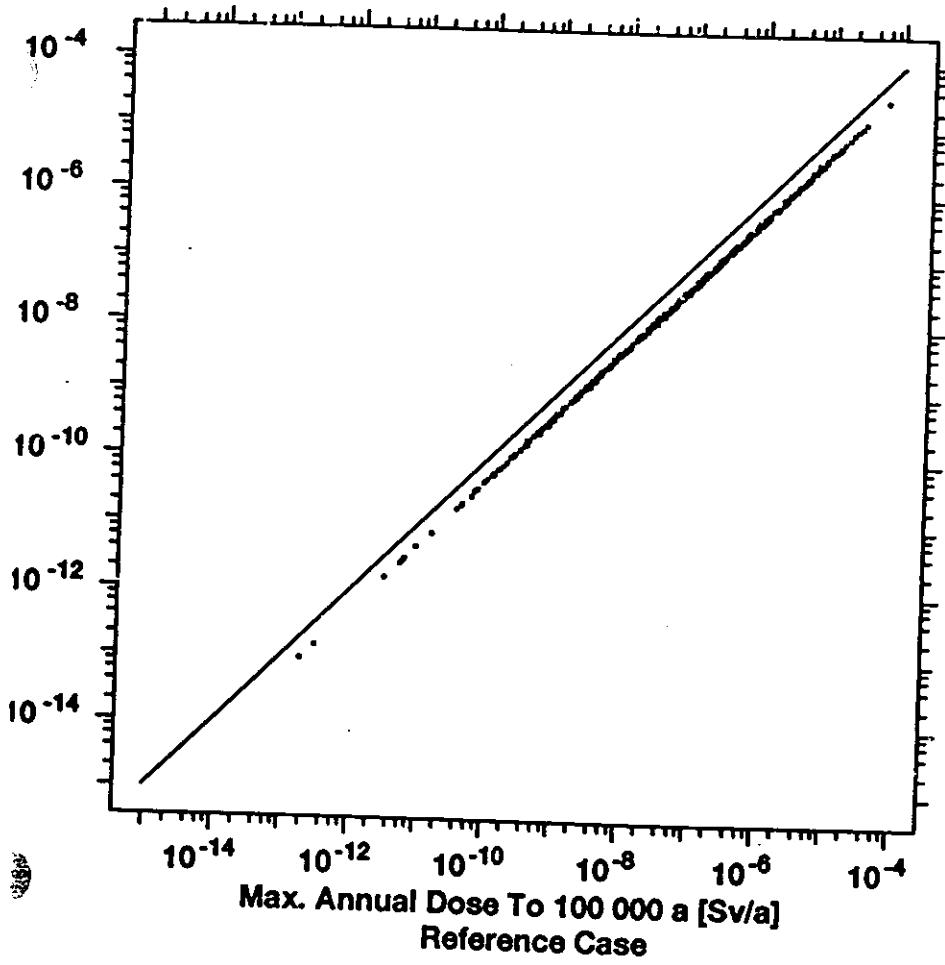
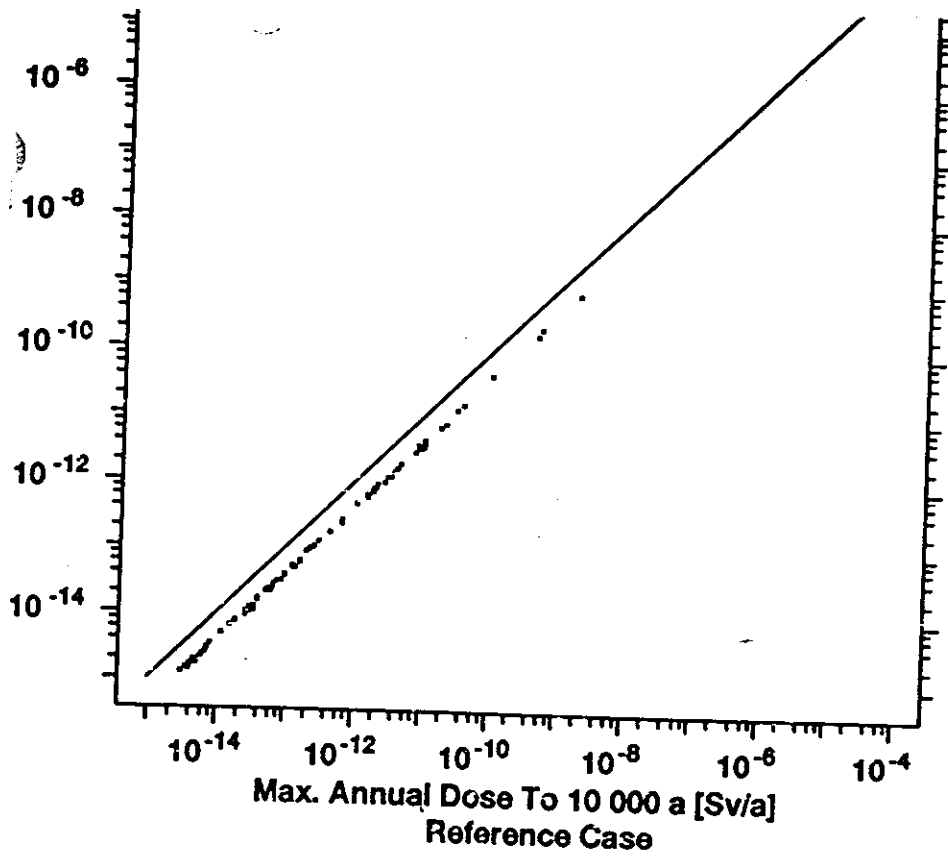


FIGURE E-42: Effect of Increased Container Wall Thick

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) (part b). Each symbol plots the results from two simulations that are identical except for the container. The horizontal axes show maximum ADEs from the reference case and the vertical axes also show maximum ADEs but taken from 500 randomly sampled simulation results. Points follow the diagonal line, indicating that the maximum ADEs are similar for both simulation types.



E-45: Effect of Increased Backfill Thickness

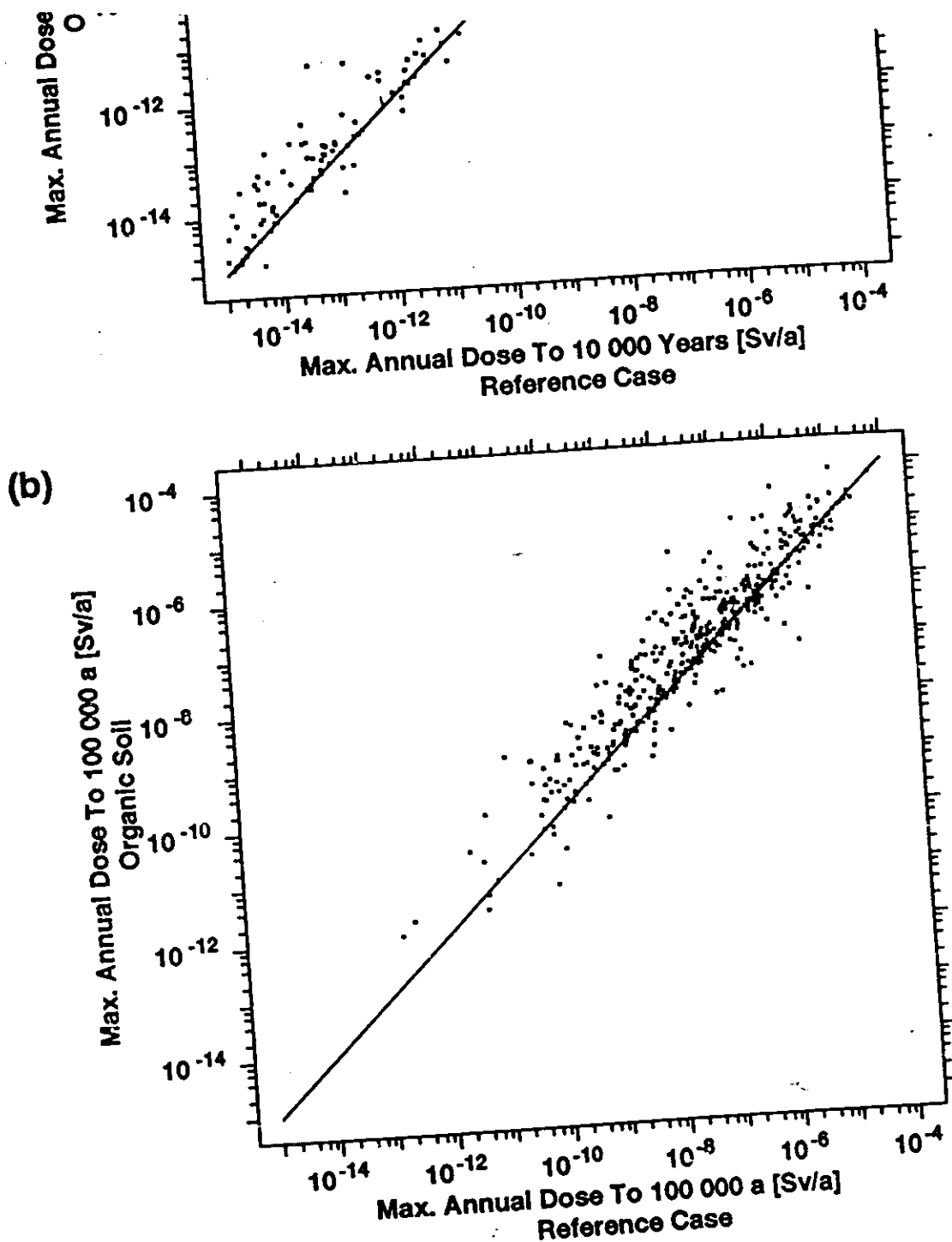
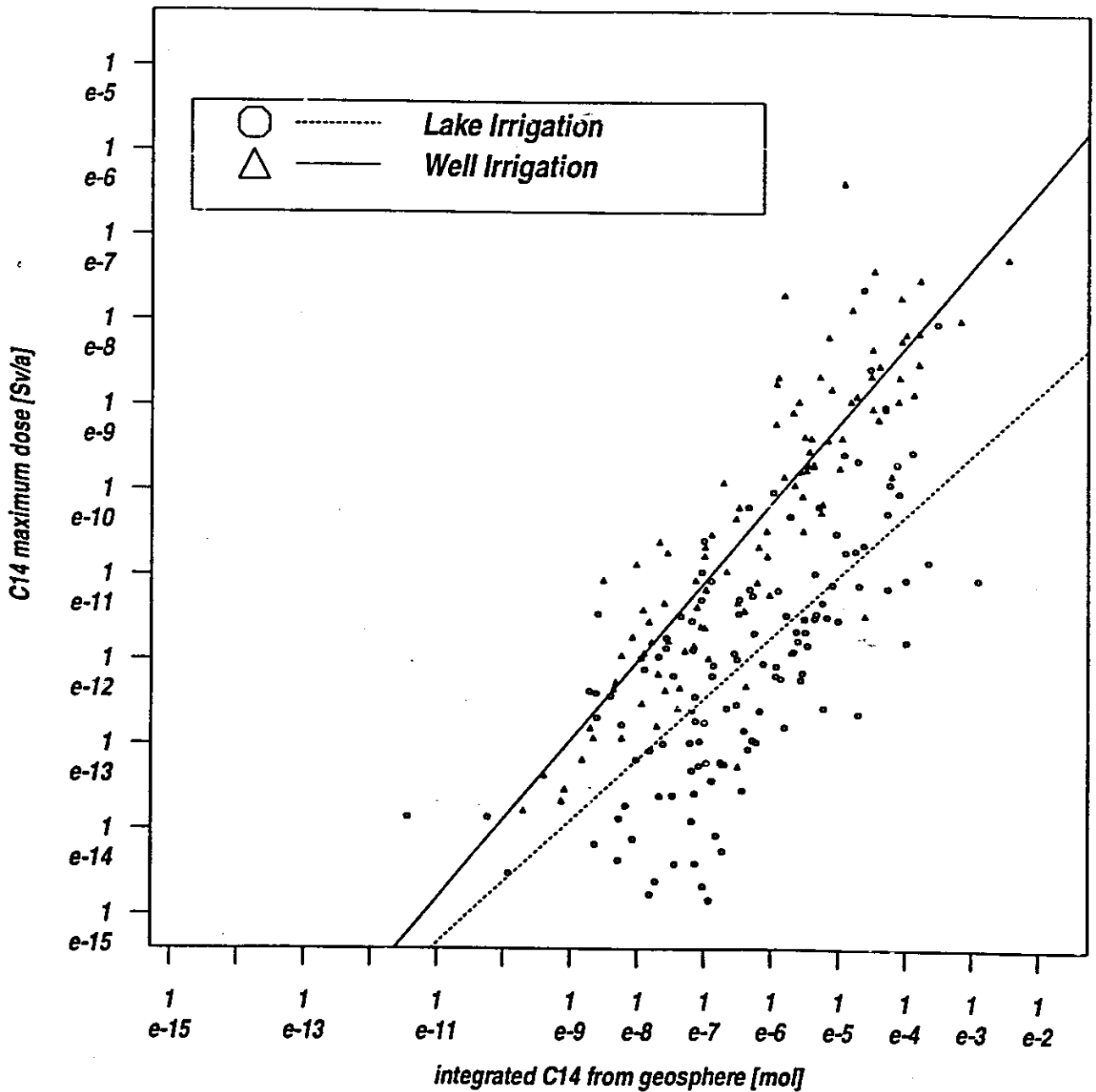
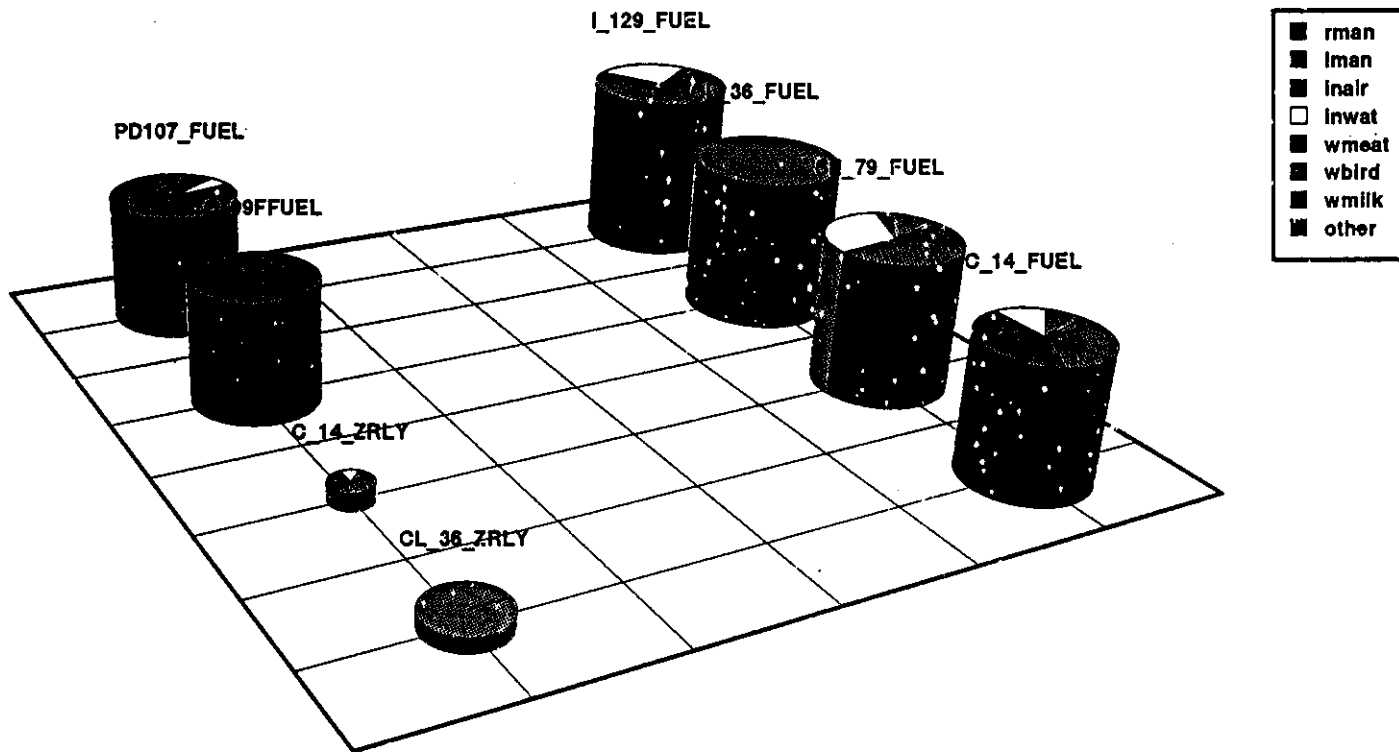


FIGURE E-53: Effect of Soil Type

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and (part b). Each symbol plots the results from two simulations that are identical except for the soil type used in the garden (and other fields) used by the critical group. The horizontal axes show the results from the reference disposal system, in which the selected soil type is sand, loam, clay or organic soil. The vertical axes show the results from 500 randomly sampled simulations where the assumed soil type is sand, loam, clay or organic soil. The diagonal line indicates that the maximum ADEs are the same for both simulations. Points falling on the diagonal line indicate pairs of simulations with identical results. Points above the diagonal line indicate simulations with larger maximum ADEs.

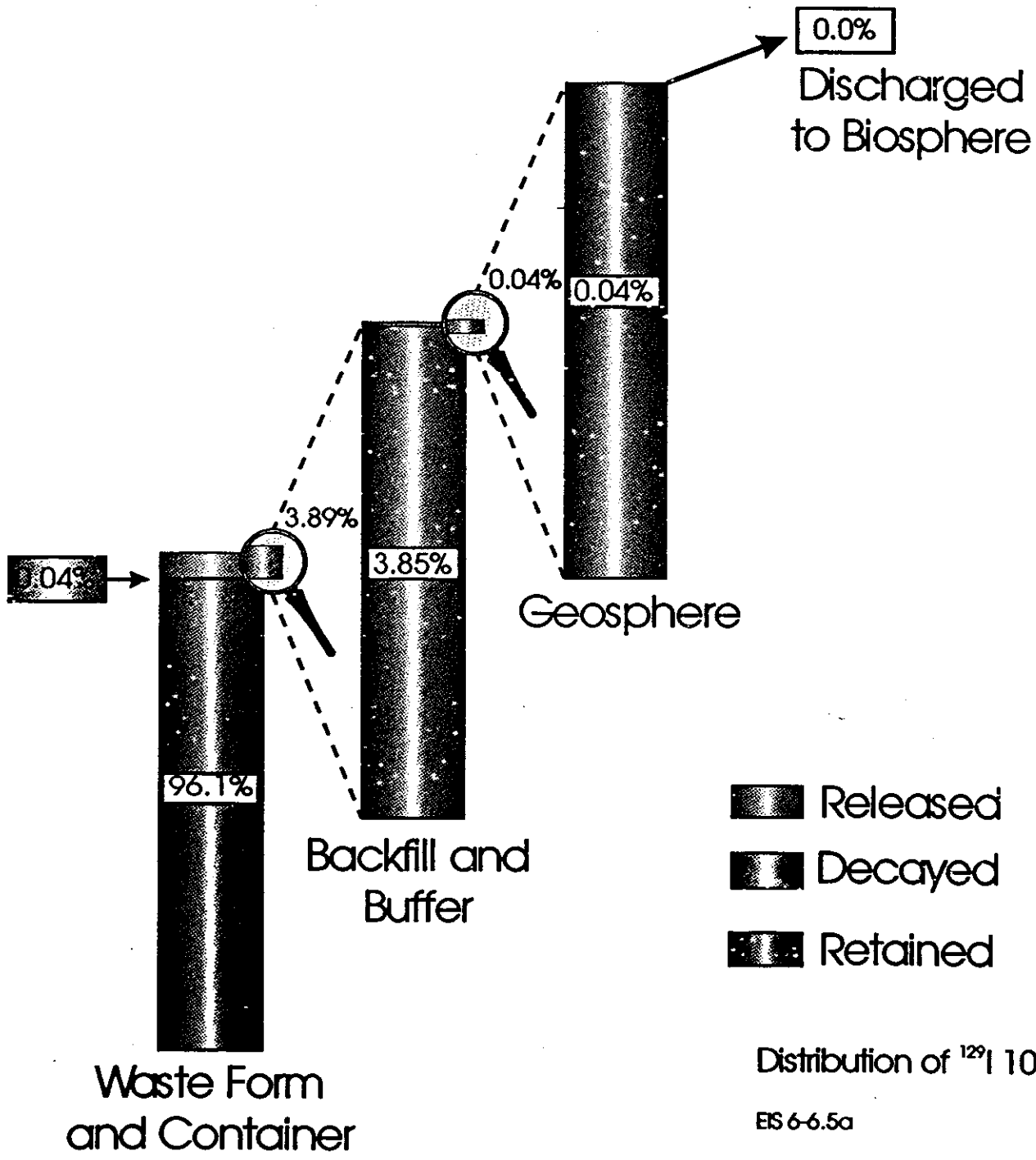
Dose from C-14 - All Pathways Simulations with Irrigated Vegetable Patch



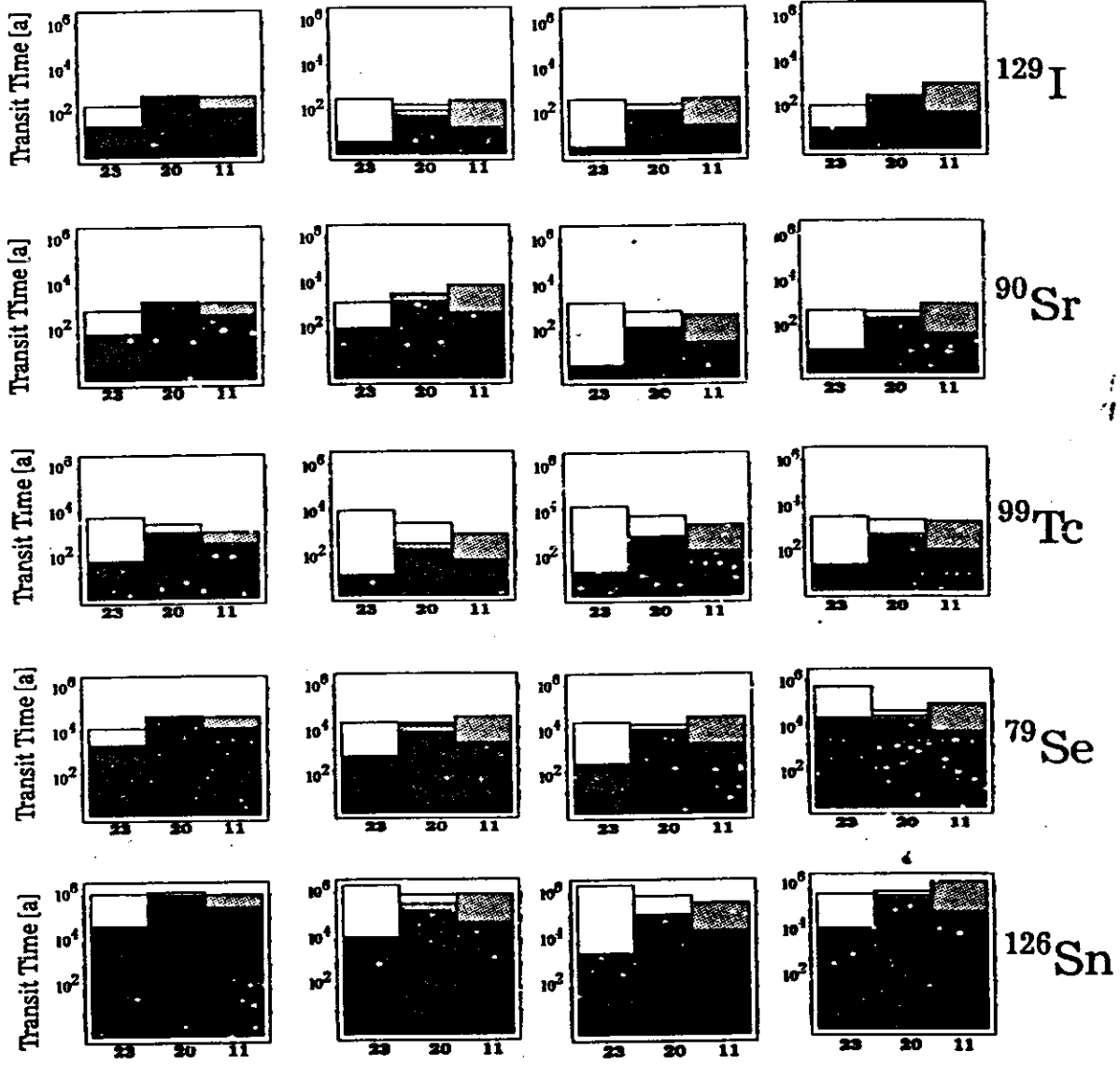


ESASSHR:[PR4INT.CNG05.RUNS.AA03_03]PR4AA03.P03
 nuclides > 1e-20
 height <- log(maximum dose)
 area <- log(integrated dose)

^{14}C	6×10^{-2}	4×10^{-2}	3×10^{-4}	2×10^{-6}	7×10^{-9}
^{129}I	6×10^{-2}	6×10^{-2}	6×10^{-3}	3×10^{-4}	3×10^{-4}
^{99}Tc	6×10^{-2}	6×10^{-2}	1×10^{-14}	2×10^{-17}	2×10^{-17}
^{90}Sr	5×10^{-4}	5×10^{-12}	9×10^{-14}	0	0
^{39}Ar	8×10^{-2}	6×10^{-6}	5×10^{-11}	3×10^{-30}	4×10^{-31}
^3H	0.3	4×10^{-12}	6×10^{-21}	0	0
Sb	8×10^{-9}	8×10^{-9}	2×10^{-13}	9×10^{-15}	9×10^{-15}
Br	7×10^{-2}	7×10^{-2}	6×10^{-3}	3×10^{-4}	3×10^{-4}
^{239}Pu	3×10^{-9}	3×10^{-9}	3×10^{-18}	0	0



MV Simulation Simulation 27 Simulation 31 Simulation 3



From Vault Sector #

Lower Fracture Zone
 Middle Rock Zone
 Lower Rock Zone

Modelling using DE's

- ◆ solve linear DE for impulse input
- ◆ use convolution to get final solutions
- ◆ SYVAC3 has a Math Library of linear DE solutions
- ◆ SYVAC3 has time series operations for convolutions, including handling chain member precursors
- ◆ Modelling with the SYVAC3 tools is a big advantage

DIFFERENTIAL EQUATION SET

$$K_i \frac{\partial R_i}{\partial t} = -V \frac{\partial R_i}{\partial x} + D \frac{\partial^2 R_i}{\partial x^2} - K_i \lambda_i R_i + K_{i-1} \lambda_{i-1} R_{i-1} \quad i = 1, n$$

with initial condition

$$R_i(x, 0) = 0, \quad i = 1, n$$

and boundary condition

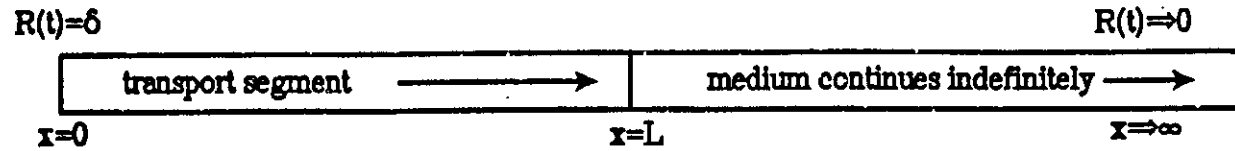
$$R_i(0, t) = \delta_i, \quad i = 1$$

$$R_i(0, t) = 0, \quad i > 1$$

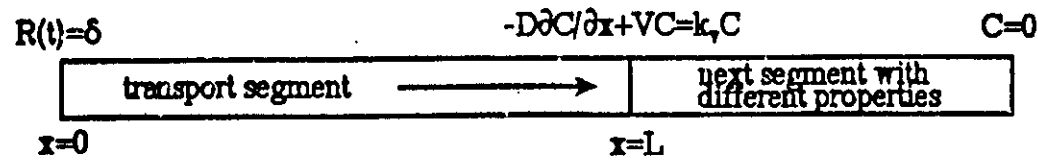
$$\lim_{x \rightarrow \infty} R_i(x, t) = 0, \quad i = 1, n$$

Solution published: Heinrich and Andres,
Ann. Nucl. Energy, 12, 685, (1985)

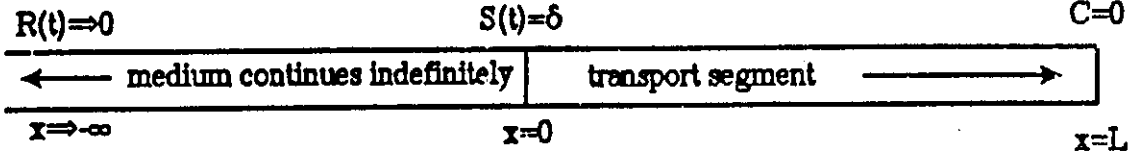
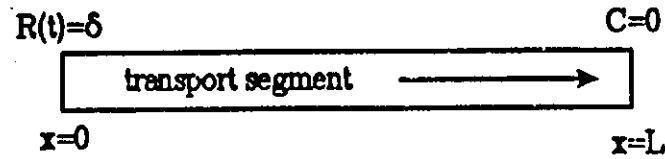
Semi-infinite medium



Mass transfer coefficient



Zero Concentration



Source within medium

$$O_{ij}(t) = \int_0^t I_i(t') R_{ij}(t-t') dt'$$

$$O_j(t) = \sum_i O_{ij}(t)$$

TIME SERIES OPERATIONS

Convolution with a Response Function

Linear systems with time-dependent inputs and outputs can be solved using convolution. The figure shows an impulse input and the output response of a linear system.

Value

Input impulse

Response function

Time

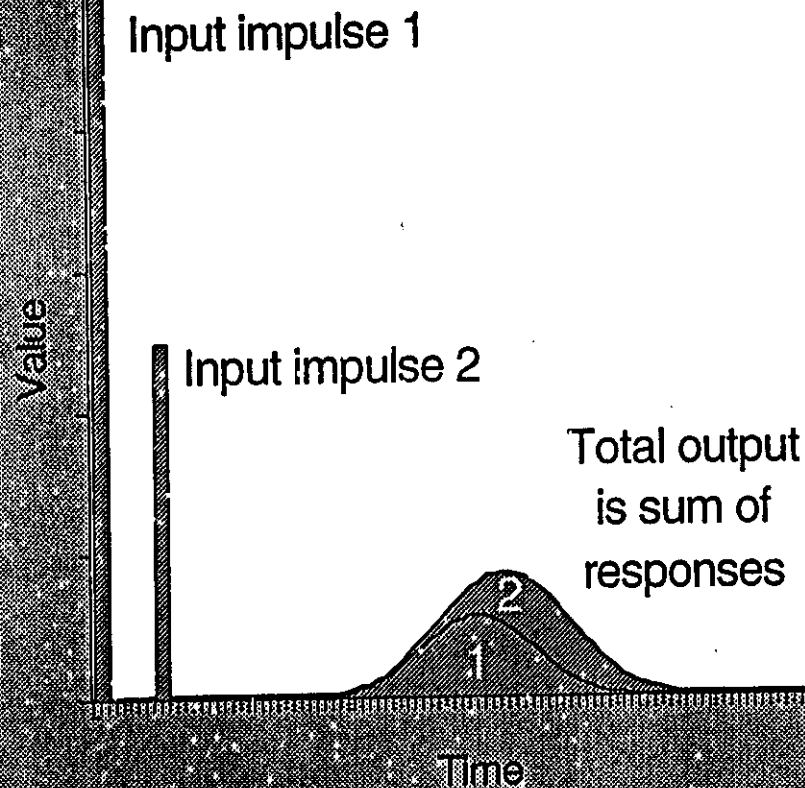
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TIME SERIES OPERATIONS

Responses can be Added

The area of a response function varies with the size of the impulse input. Responses can be added together to yield the total system response to multiple inputs.



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TIME SERIES OPERATIONS

Convolution Integrates Output

Convolution is a mathematical way of breaking up any input into impulses, and of adding the responses to find the total system output.

Value

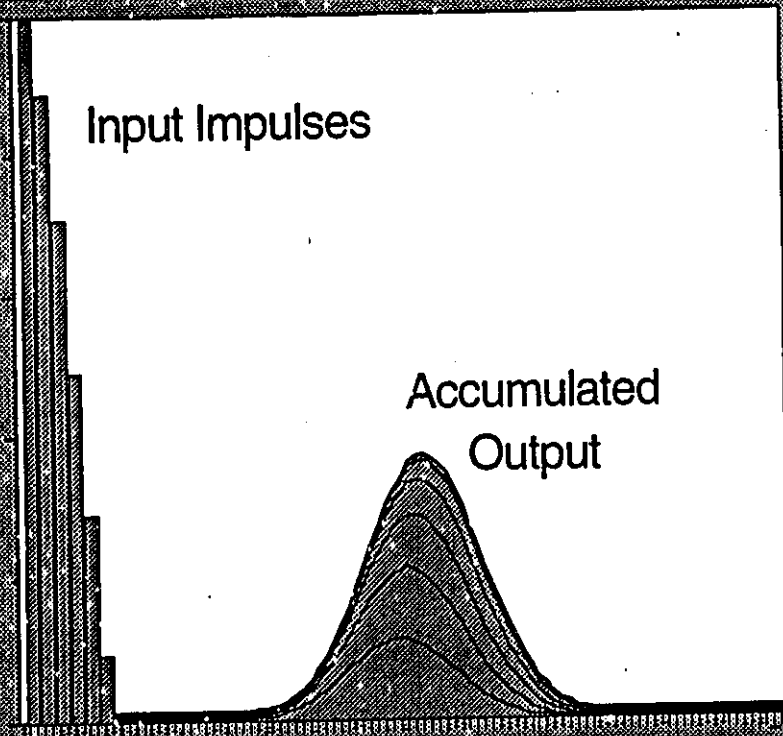
Input Impulses

Accumulated Output

Time

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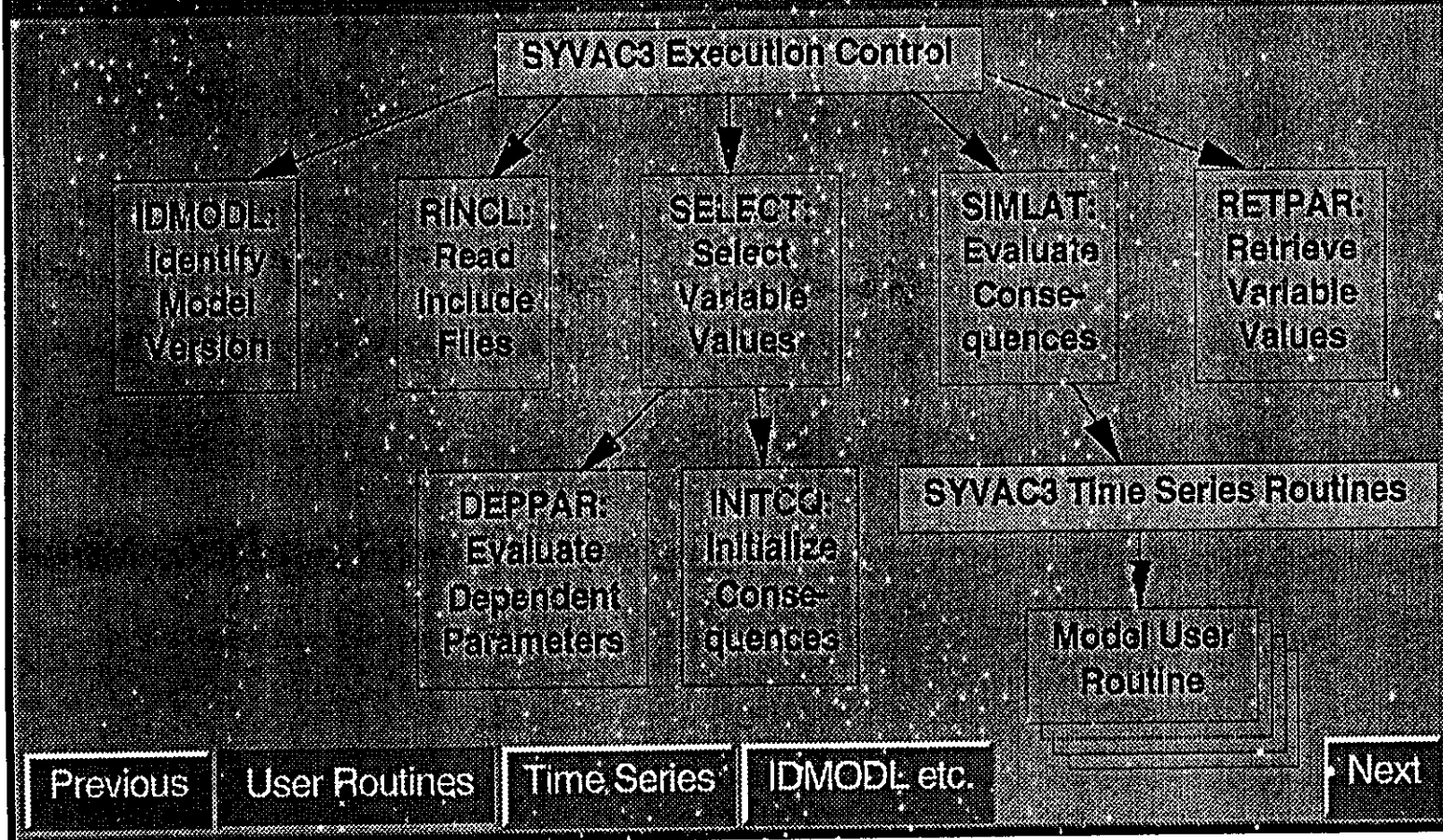


Interfaces to System Models

- ◆ 7 interface modules
- ◆ 5 have standard forms from templates
 - model identification
 - initializing and passing parameters to/from input and output
- ◆ 2 for driving model execution

SYVAC3: PROGRAMMER'S VIEW

Standard Model Interface Routines



INTERFACE ROUTINES

Called by SYVAC3 to Activate a Model

IDMODL: Return a two-character model identifier

RINCL: Read include files to identify variables

SELECT: Assign parameters, initialize consequences

DEPPAR: Evaluate dependent parameters

INITCQ: Initialize consequence variables

SIMLAT: Evaluate simulation consequences

RETPAR: Retrieve variable values for output

Return

Next

Linking to Models

- ◆ Any FORTRAN coded model can be embedded into SYVAC3 for control of execution in a probabilistic/deterministic framework
- ◆ must use a standard SYVAC3 format for input/output variable common blocks
- ◆ Other models can be interfaced also by linking SYVAC3 to only their input files and running them externally

INTERFACE ROUTINES

Why does SYVAC3 Read Model Code?

SYVAC3 reads part of the model code, specifically the include files where model variables are declared. Why?

To find out where to:

- store the values of sampled parameters
- initialize consequence variables
- retrieve the values of all model variables at the end of each simulation

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INTERFACE ROUTINES

Effects of SYVAC3 Reading Code

Because SYVAC3 reads the model include files containing model variable declarations (SPxxxx, CQxxxx, DPxxxx):

- the include files must be present in the directory where SYVAC3 is run
- the include files must be written in a conventional way
- if array declarations use Fortran parameters for array bounds, these must be defined for SYVAC3
- several interface routines include some or all of the include files

[Previous](#)

[Main Text](#)

INTERFACE ROUTINES

Recommended Include File Format

INTEGER LSABCD	
PARAMETER (LSABCD = 1+MXSPEC)	length of common block
DOUBLE PRECISION	
1 SPABCD(LSABCD)	vector of same length
DOUBLE PRECISION	
1 PARM1,	first parameter []
1 PARM2	vector []
COMMON /SPABCD/	
1 PARM1,	
1 PARM2(MXSPEC)	dimension here
EQUIVALENCE (PARM1,SPABCD(1))	two ways to access data

[Previous](#)

[Main Text](#)