Section 4

Sensitivity Analysis

and

SYVAC3 applications

OBJECTIVES OF SENSITIVITY ANALYSIS

- develop derived constraints
- set research priorities
- test models and data
- develop better models and data
- develop a simple description of the system

CLARIFIED DESCRIPTION

- identify important

  parameters
  radionuclides
  pathways
  barriers
  features

- show how they affect performance

METHODS USED WITH SYVAC3-CC3

- screening
- detailed cause-effect study
- exceptional analysis

SCREENING ANALYSIS

based on

- **expert knowledge**
- **"conventional" methods**
- **iterated fractional factorial design**

Simulation Number	Parameter P1	P2	P3	P4	P5	P6	P7	P8	Result of simulation
1	H	H	H	H	H	H	H	H	H
2	H	L	H	L	H	L	H	L	H
3	H	H	L	L	H	H	L	L	L
4	H	L	L	H	H	L	L	H	L
5	H	H	H	H	L	L	L	L	H
6	H	L	H	L	L	H	L	H	H
7	H	H	L	L	L	L	H	H	L
8	H	L	L	H	L	H	H	L	L
9	L	L	L	L	L	L	L	L	L
10	L	H	L	H	L	H	L	H	L
11	L	L	H	H	L	L	H	H	H
12	L	H	H	L	L	H	H	L	H
13	L	L	L	L	H	H	H	H	L
14	L	H	L	H	H	L	H	L	L
15	L	L	H	H	H	H	L	L	H
16	L	H	H	L	H	L	L	H	H

EXPERIMENT 3: 8 COINS

OBSERVATION 1: 1-H 2-H 3-H 4-H 5-H 6-H 7-H 8-H EFFECT:________
OBSERVATION 2: 1-H 2-H 3-H 4-T 5-H 6-T 7-T 8-T EFFECT:________
OBSERVATION 3: 1-H 2-H 3-T 4-H 5-T 6-H 7-T 8-T EFFECT:________
OBSERVATION 4: 1-H 2-H 3-T 4-T 5-T 6-T 7-H 8-H EFFECT:________

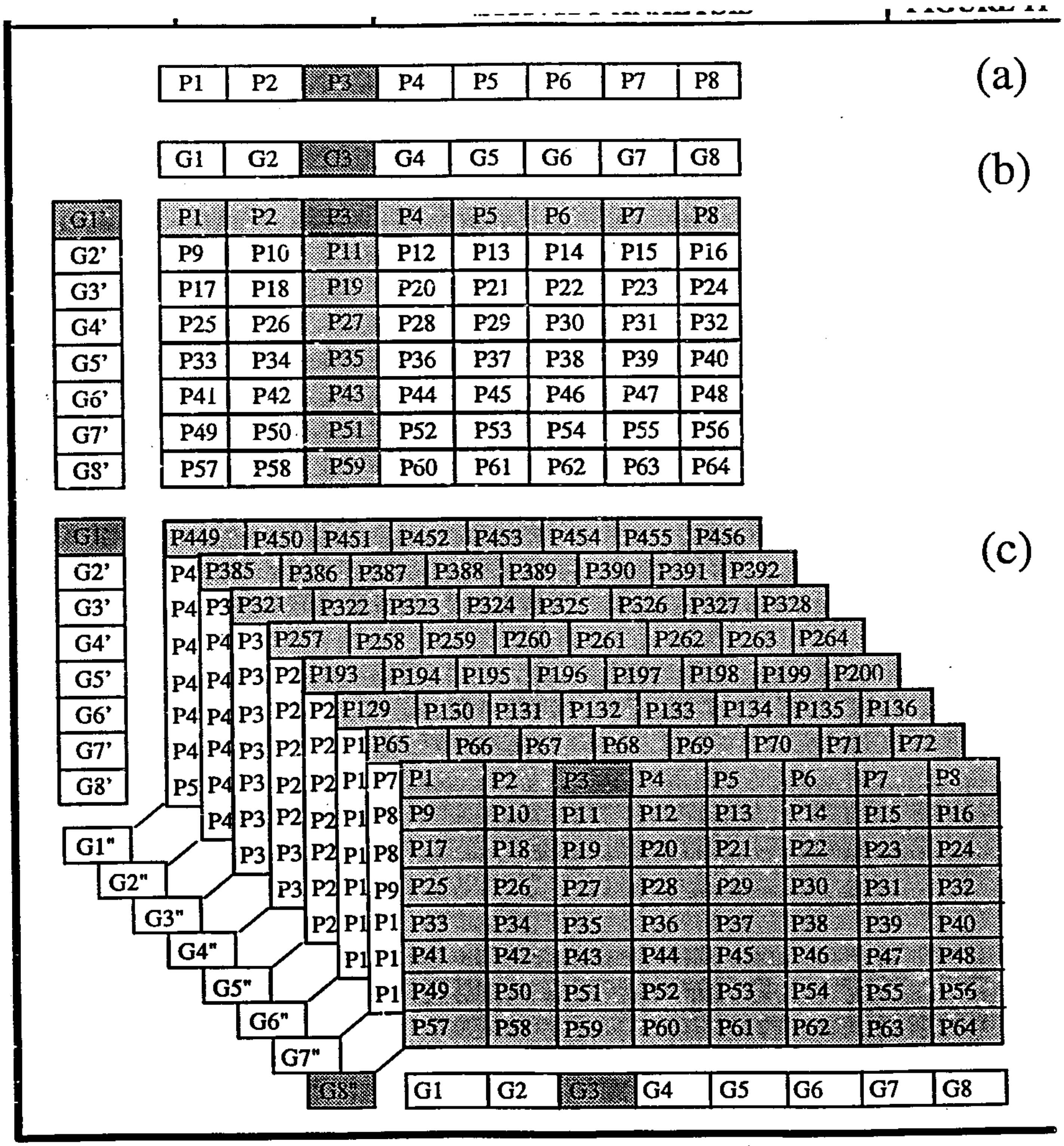
OBSERVATION 5: 1-H 2-T 3-H 4-H 5-T 6-T 7-H 8-T EFFECT:________
OBSERVATION 6: 1-H 2-T 3-H 4-T 5-T 6-H 7-T 8-H EFFECT:________
OBSERVATION 7: 1-H 2-T 3-T 4-H 5-H 6-T 7-T 8-H EFFECT:________
OBSERVATION 8: 1-H 2-T 3-T 4-T 5-H 6-H 7-H 8-T EFFECT:________

OBSERVATION 9: 1-T 2-T 3-T 4-T 5-T 6-T 7-T 8-T EFFECT:________
OBSERVATION 10: 1-T 2-T 3-T 4-H 5-T 6-H 7-H 8-H EFFECT:________
OBSERVATION 11: 1-T 2-T 3-H 4-T 5-H 6-T 7-H 8-H EFFECT:________
OBSERVATION 12: 1-T 2-T 3-H 4-H 5-H 6-H 7-T 8-T EFFECT:________

OBSERVATION 13: 1-T 2-H 3-T 4-T 5-H 6-H 7-T 8-H EFFECT:________
OBSERVATION 14: 1-T 2-H 3-T 4-H 5-H 6-T 7-H 8-T EFFECT:________
OBSERVATION 15: 1-T 2-H 3-H 4-T 5-T 6-H 7-H 8-T EFFECT:________
OBSERVATION 16: 1-T 2-H 3-H 4-H 5-T 6-T 7-T 8-H EFFECT:________

EFFECT OF COIN 1: H-AVG ______ - T-AVG ______ = ______
EFFECT OF COIN 2: H-AVG ______ - T-AVG ______ = ______
EFFECT OF COIN 3: H-AVG ______ - T-AVG ______ = ______
EFFECT OF COIN 4: H-AVG ______ - T-AVG ______ = ______

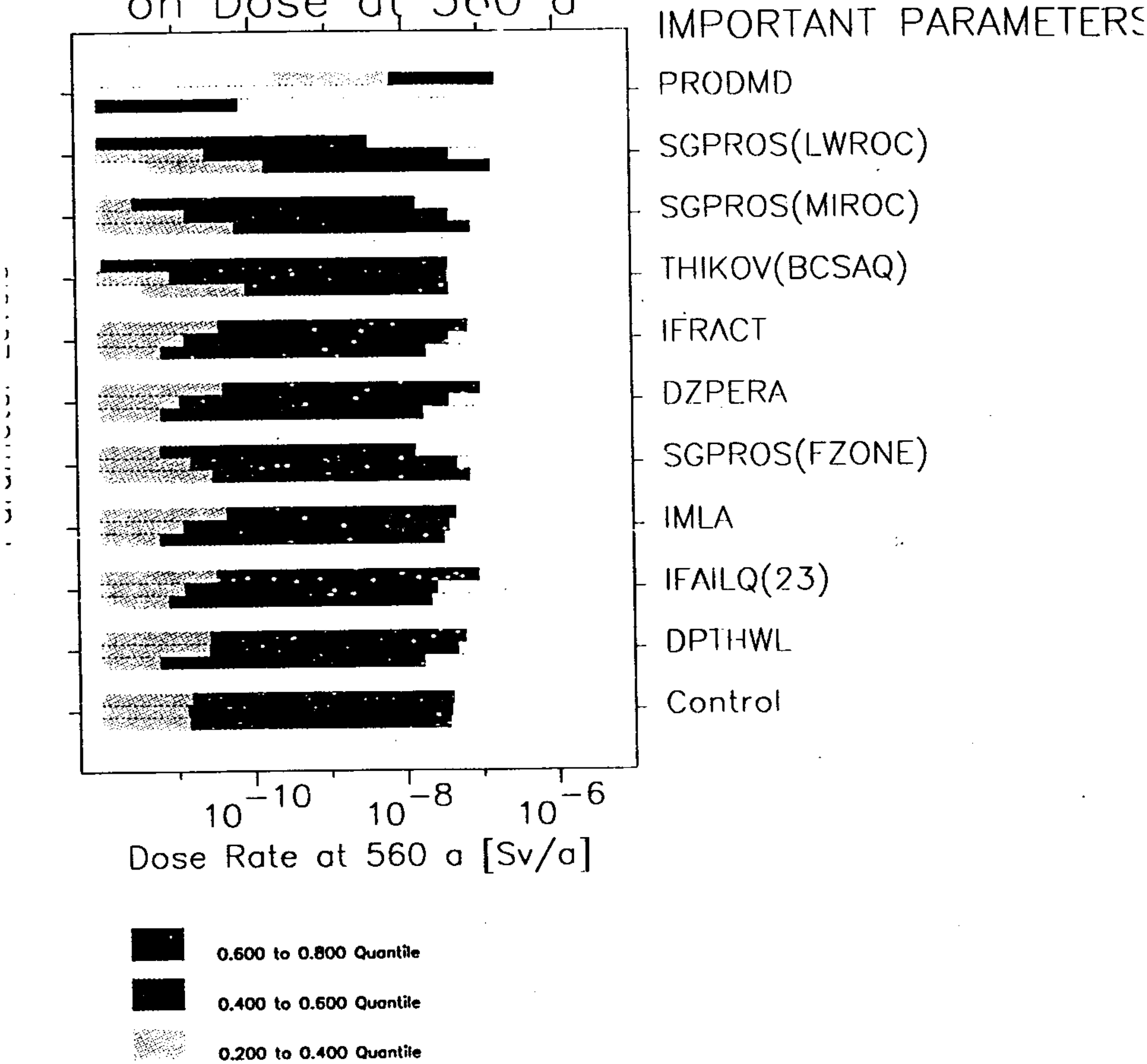
EFFECT OF COIN 5: H-AVG ______ - T-AVG ______ = ______
EFFECT OF COIN 6: H-AVG ______ - T-AVG ______ = ______
EFFECT OF COIN 7: H-AVG ______ - T-AVG ______ = ______
EFFECT OF COIN 8: H-AVG ______ - T-AVG ______ = ______


(a)
P1 P2 P3 P4 P5 P6 P7 P8
(b)
G1 G2 G3 G4 G5 G6 G7 G8
G1' G2' G3' G4' G5' G6' G7' G8'
P1 P2 P3 P4 P5 P6 P7 P8
P9 P10 P11 P12 P13 P14 P15 P16
P17 P18 P19 P20 P21 P22 P23 P24
P25 P26 P27 P28 P29 P30 P31 P32
P33 P34 P35 P36 P37 P38 P39 P40
P41 P42 P43 P44 P45 P46 P47 P48
P49 P50 P51 P52 P53 P54 P55 P56
P57 P58 P59 P60 P61 P62 P63 P64
(c)
G1' G2' G3' G4' G5' G6' G7' G8'
P449 P450 P451 P452 P453 P454 P455 P456
P385 P386 P387 P388 P389 P390 P391 P392
P321 P322 P323 P324 P325 P326 P327 P328
P257 P258 P259 P260 P261 P262 P263 P264
P193 P194 P195 P196 P197 P198 P199 P200
P129 P130 P131 P132 P133 P134 P135 P136
P65 P66 P67 P68 P69 P70 P71 P72
P1 P2 P3 P4 P5 P6 P7 P8
P9 P10 P11 P12 P13 P14 P15 P16
P17 P18 P19 P20 P21 P22 P23 P24
P25 P26 P27 P28 P29 P30 P31 P32
P33 P34 P35 P36 P37 P38 P39 P40
P41 P42 P43 P44 P45 P46 P47 P48
P49 P50 P51 P52 P53 P54 P55 P56
P57 P58 P59 P60 P61 P62 P63 P64
G1" G2" G3" G4" G5" G6" G7" G8"
G1 G2 G3 G4 G5 G6 G7 G8

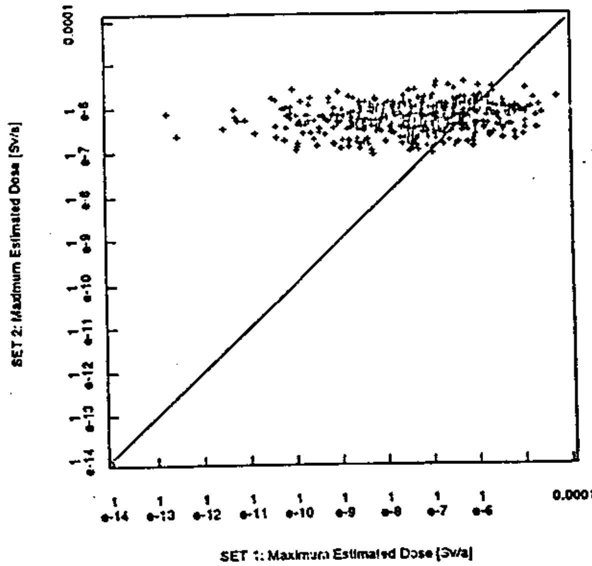
Fractional Factorial Sensitivity Analysis

index	Parameters	2 level full design	2 level Res IV fractional factorial	Iterated Fractional Factorial (based on 8 groups)
n	P = 8^n	2^P	2P	16n
1	8	256	16	16
2	64	1.8E19	128	32
3	512	1.3E154	1024	48
4	4096	--	8192	64
5	32768	--	65536	80

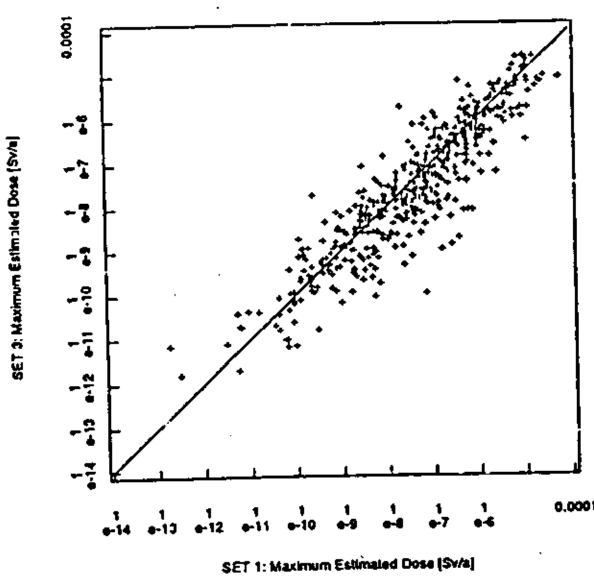
fect of Important Parameters on Dose at 560 a

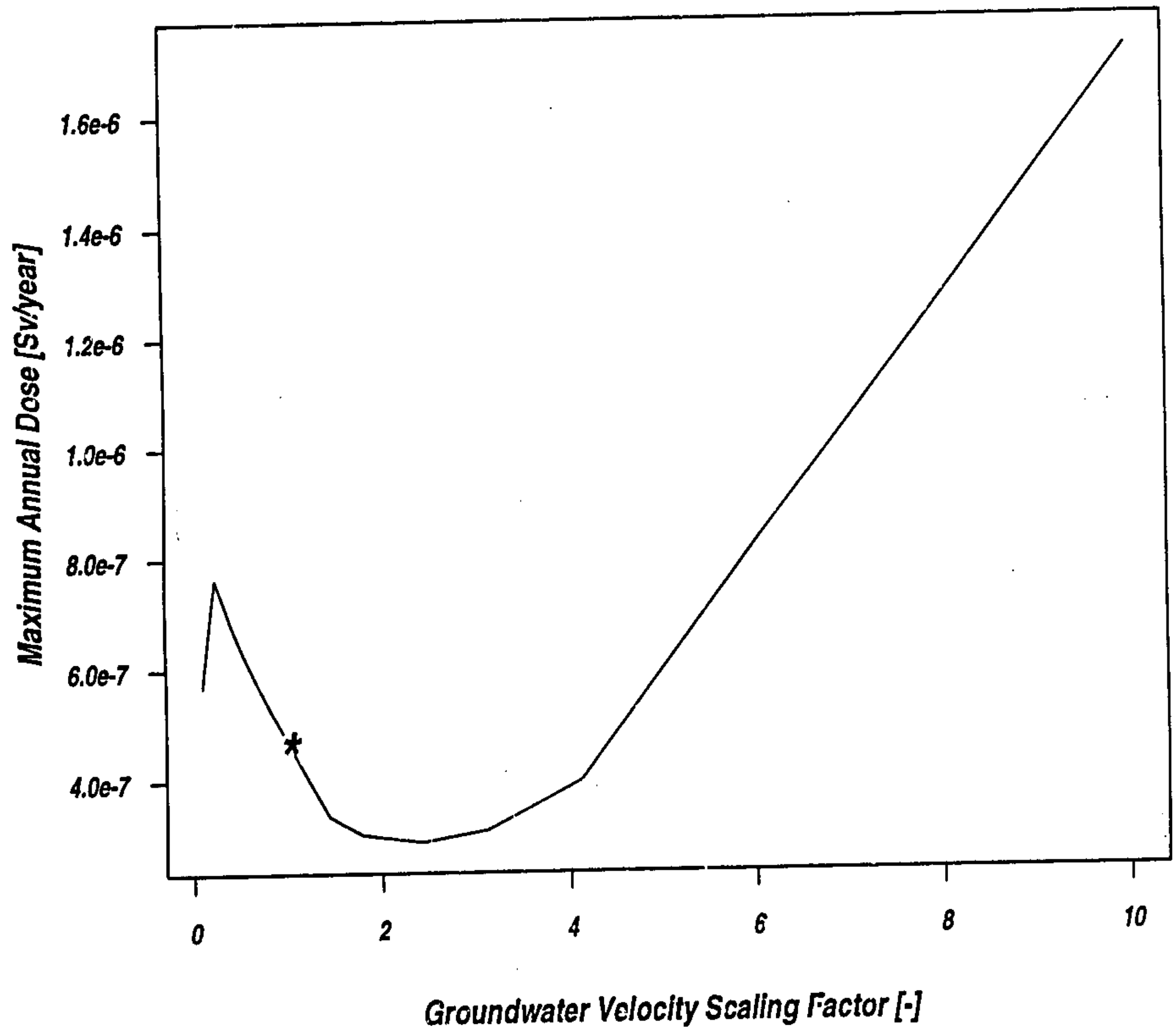


Effect of holding 'studied' parameters constant

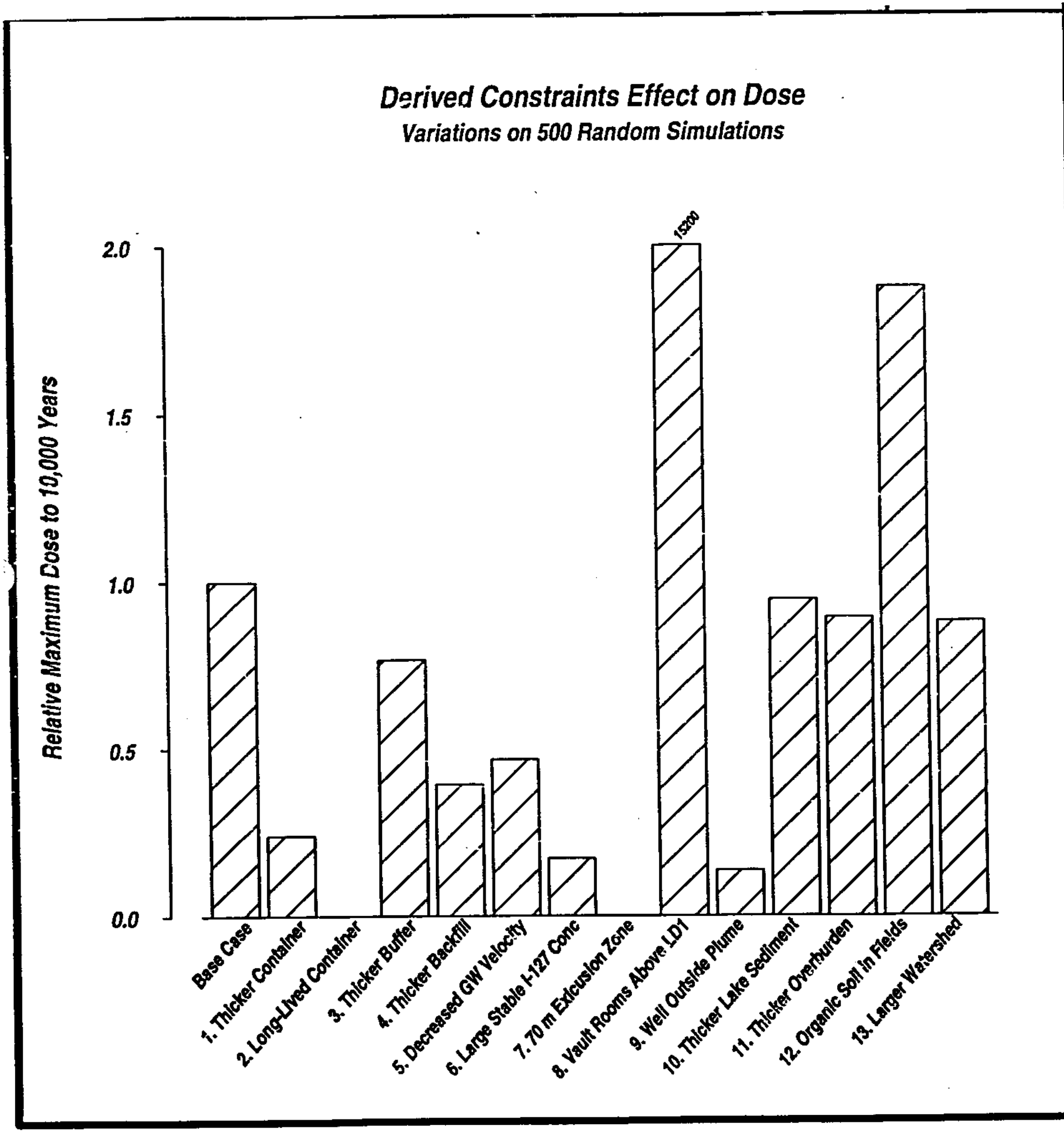


Effect of holding 'unstudied' parameters constant





1.6e-6
1.4e-6
1.2e-6
1.0e-6
8.0e-7
6.0e-7
4.0e-7
Maximum Annual Dose [Sv/year]
0
2
4
6
8
10
Groundwater Velocity Scaling Factor [-]


Derived Constraints Effect on Dose
Variations on 500 Random Simulations
Relative Maximum Dose to 10,000 Years
2.0
1.5
1.0
0.5
0.0
15200
Base Case
1. Thicker Container
2. Long-Lived Container
3. Thicker Buffer
4. Thicker Backfill
5. Decreased GW Velocity
6. Large Stable I-127 Conc
7. 70 m Exclusion Zone
8. Vault Rooms Above LD1
9. Well Outside Plume
10. Thicker Lake Sediment
11. Thicker Overburden
12. Organic Soil in Fields
13. Larger Watershed

EVOLUTION OF SYVAC

- SYVAC1 (1981)
  - study Systems Variability Analyses method
- SYVAC2 (1985)
  - examine complex models
- SYVAC3 (1986 -)
  - simplify model addition

SYVAC1 APPLICATIONS

- ICAD1, CNFWM concept
  (Wuschke et al 1981)

- subseabed disposal, fuel recycle
  wastes
  (Wuschke et al 1983, Guvanasen
  1987)

- Geological disposal, intermediate
  level wastes
  (Guvanasen 1985)

SYVAC2 APPLICATIONS

- **ICAD2, CNFWM concept (Wuschke et al 1985)**
- **chemical toxicity, CNFWM concept (Goodwin et al 1987)**

SYVAC3 APPLICATIONS

- QA of UTAP (tailings)
  (Goodwin et al 1986, 1987)

- PSAG code intercomparisons
  (NEA, 1987, 1989, 1990)

- Geological disposal, low level
  wastes
  (ACRES, 1989)

SYVAC3 applications cont'd

- Scottish Nuclear
  - high level nuclear waste geological disposal
- Canadian Low Level & Intermediate Level Radwaste
  - Michigan Basin site in Central Canada with Ontario Hydro waste inventories
  - Chalk River site with AECL waste inventories

SYVAC3 applications cont'd

- Externally run programs
  - SYVAC3 sampling used to generate input file for an external program (no embedded model)
  - Input files are run in external program and results analysed in same way
  - CATHENA - reactor safety analysis code
  - MOTIF - FE groundwater flow modelling code

1. INTRODUCTION

The Canadian Concept, generation 3 (CC3), GEOsphere NETwork model, GEONET, describes the movement of contaminants, released from an underground disposal vault, through the geosphere. GEONET represents a geological system by a network of one-dimensional transport segments joined together in three-dimensional space. It tracks the movement of contaminants released from the system of engineered barriers of the vault to their ultimate discharge into the surface environment. The specifications in this report define the geosphere model, which is coded in FORTRAN-77 and installed as part of the CC3 models (version 05) used with an executive program, SYVAC3 (version 09) for the postclosure assessment of the concept for disposal of nuclear fuel waste (Goodwin et al. 1994). The executive code SYVAC3 (Systems Variability Analysis Code, generation 3) (Goodwin et al. 1987) provides a platform for probabilistic analysis to account for uncertainties in simulation of the performance of a disposal system.

The network representation of the geosphere provides a flexible approach that is easily adapted to a wide variety of geological systems. The network incorporates the lithostructural features, fracture framework, groundwater flow paths, and mineralogical and geochemical conditions that characterize a geological system. GEONET has been used in a postclosure assessment case study of a hypothetical disposal system (Goodwin et al. 1994) which, in turn, forms part of an Environmental Impact Statement (AECL 1994). In this case study, GEONET has been applied to the Whiteshell Research Area (WRA), a field study area in Southeastern Manitoba. The WRA has been the subject of intensive field investigations, including those necessary to locate and construct an Underground Research Laboratory.

A description of the geosphere model is presented in a primary reference for the Environmental Impact Statement (EIS) entitled "The Disposal of Canada's Nuclear Fuel Waste: The Geosphere Model for Postclosure Assessment" (Davison et al. 1994). Portions of Chapters 6 and 7 of this primary reference have been reproduced, with only minor changes, in Chapter 4 of this report. Equation numbers have been left the same as in the original document, starting with numerals "6" or "7", for easier cross referencing. An additional section, numbered 4.3, that does not appear in the primary reference, has been added to Chapter 4, with equation numbers starting with numeral "4", to describe the details of the implementation of matrix diffusion effects.

The general principles upon which a set of specifications is based have been clearly stated by others:

> "The specification should contain all the true requirements and nothing but the true requirements . . . A true requirement is a feature or capability that a system must possess in order to fulfill its purpose, regardless of how the system is implemented." (McMenamin and Palmer 1984, p. 3)

> ". . . a good specification ought to be clear, unambiguous, concise (to avoid excessive volume), and complete (so that no essential element is left unspecified) . . . it should

state what has to be accomplished by the system rather than how the system should accomplish it." (DeMarco 1978, p. 169).

Thus, a good specification states what the transformation is, without detailing how the transformation is to be implemented.

These specifications are written in a form generally referred to as Yourden-DeMarco (DeMarco 1978; Yourden 1989) and consist of data flow diagrams, minispecifications, and a data dictionary. The format of these components is described in Chapter 2. Specific conventions followed by this set of geosphere model specifications are given in Chapter 3. A description of the geosphere model and its application to the VRA is given in Chapter 4. The specifications themselves are given in Chapter 7 for the Data Flow Diagrams, Chapter 8 for the Minispecs and Chapter 9 for the Data Dictionary. In order to make navigation and reading of the specifications easier, Chapter 5 gives several indexed listings, cross referencing each subcomponent of the specifications, and Chapter 6 gives a summary of the contents of composite data flows and data stores together with definitions of variables used as indices.

2. FORMAT FOR CC3 MODEL SPECIFICATIONS

Formal specifications for the SYVAC3-CC3 models consist of three components:

1. data flow diagrams (DFDs),
2. minispecifications (minispecs), also called data dependency diagrams (DDDs), and a
3. data dictionary (DD).

The following notes describe the format of each.

2.1 DATA FLOW DIAGRAMS (DFDs)

A DFD is a network representation of a system, and shows the actions of the system (processes) and the data interfaces between them (data flows). It is also commonly referred to as a "Bubble Diagram" because the processes are represented by circles or "bubbles". The diagram conventions outlined below are used.

2.1.1 Overall Structure

A complete model is represented by a set of DFDs. The highest-level DFD, called Diagram -1, the Context Diagram, shows all interactions of the modelled system with the world outside of the system. The top level DFD, called Diagram 0, represents the entire system at a general level. Bubbles (circles) represent processes, and arrows represent data flows between processes. Each bubble in Diagram 0 may be expanded into another full DFD representing more detailed data flows and processes. Bubbles appearing on detailed DFD's may again be expanded into more detailed DFDs. This expansion occurs successively, until the processes are simple enough to be described by a minispec (see Section 2.2). The bubbles are numbered to show the successive expansions. Bubbles shown in Diagram 0 are numbered 1, 2, 3, etc. Bubbles shown in Diagram 2, which is an expansion of bubble 2 on Diagram 0, are numbered 2.1, 2.2, 2.3, etc. Those in Diagram 2.3, an expansion of bubble 2.3 on Diagram 2, are numbered 2.3.1., 2.3.2, 2.3.3, etc. All bubbles are labelled or named to indicate the process represented (as described in Section 2.1.2).

2.1.2 Processes

All bubbles are labelled or named with unique verb phrases. A bubble may have any number of incoming and outgoing data flows. If a bubble has only one outflow, it is usually named "Calculate...". Otherwise, a more general name is used. Bubbles are also labelled with unique numeric identifiers, like "1.3.2" (the meaning of the sequence of numeric identifiers is explained above in Section 2.1.1).

2.1.3 Data Flows

All variables needed in a process are shown as data flows entering the appropriate bubble. Variables that are explicitly calculated emerge from a bubble. Data flows coming from the edge of a DFD are variables that were generated on another DFD and their origin can be traced on the higher-level diagram. Data flows leading to the edge of the DFD are variables that will be used in another DFD, and their destinations can be traced on the higher-level diagram. The top-level DFDs, Diagrams -1 and 0, show all the input parameters that are used in the model and their sources from outside the system.

Each data flow is given a unique name. Different styles of arrowed lines are used to distinguish data flows that are not functions of time from those that are functions of time. An asterisk next to the name of a data flow means that the data flow appears more than once in the same DFD.

To prevent clutter, parameters may be grouped together in a list called a composite data flow. This composite data flow may be expanded at lower levels into its components. When such a composite data flow is expanded, a note is placed on the diagram on which the expansion occurs, indicating the components of the composite data flow. In addition, the composite data flows are also defined in the data dictionary. The conventions used in the notation of the expansion are indicated in Section 2.3.8 with the description of the data dictionary.

2.1.4 Data Stores

Data produced by one process may be stored for subsequent use by another process. This is done by directing a data flow into a data store. A data store is represented by two parallel horizontal line segments. However, any data exiting must have entered from an earlier calculation. Each data store is named and the name appears between the horizontal line segments. An example of a data store use would be the storage of a nuclide flow rate such that it may be used as the precursor flow rate in the calculations for a subsequent nuclide in a decay chain. The data store names are also defined in the data dictionary with an expansion of the data items they contain. Unlabelled data flows entering and exiting a data store are flows of potentially the entire contents of the data store.

2.1.5 Notes

Any additional explanation of the diagram is given at the bottom in the form of notes. The notes are numbered sequentially for reference.

2.2 MINISPECIFICATIONS (MINISPECS)

Minispecs detail the workings of each process bubble that is not expanded into another DFD. The type of minispec currently used for the specifications of the SYVAC3 submodels is known as a data dependency diagram (DDD). It contains the components outlined below.

2.2.1 Definitions of the Outgoing Data Flows

Data flows that are calculated in a DDD for use elsewhere are defined at the top of the minispec. The definition comprises a short name, qualifiers, a long name, SI units, and the complete text definition from the Data Dictionary.

2.2.2 The Data Dependency

This field unambiguously depicts the dependencies between data fields. Two forms of this field may appear: a table, or a diagram. Both data dependency forms contain essentially the same information and are described below.

a) The tabular form is composed of a box showing separate lists of time-dependent and time-independent data flows involved in the process. There is also a table containing for each such data flow
   - the data flow name or short name,
   - a longer descriptive name or long name,
   - the mathematical symbol used in equations for the variable, and
   - the SI units.

   Entries are in alphabetical order by short name. The table can also contain an indication of whether the data flow is calculated somewhere else in the model or whether it is an input parameter.

b) The diagrammatic form comprises a labelled ellipse for every calculated variable entering the process and a labelled rectangle for every input parameter entering the process, joined by arrows showing which variables depend on which. The labels in the ellipses or rectangles consist of both the short and long names of the variable. The ellipses may also include the number of the DDD used to calculate the variable.

2.2.3 Equations

Equations or other form of instructions are given for any operations or calculations performed in the minispec. Each equation used should be numbered sequentially [e.g. Eqn. (4)]. These equations should be referenced back to the supporting documentation. Reference is made by giving the number of the equation as it appears in the supporting documentation, if possible. Where this supporting documentation uses different symbols to refer to variables, a note should be included showing the equivalences of the symbols.

2.2.4 Units Check

The units of equations are checked to ensure consistency. The units for each term and factor in the equations are shown in the minispec to show that the check was performed. Unit check equations are given numbers corresponding to the equation being checked.

2.2.5 Notes

Any additional explanation of the minispec is given at the bottom in the form of numbered notes. For example, any calculation that must occur in a specific order with respect to another, must be indicated.

2.3 DATA DICTIONARY

The data dictionary is an alphabetical list of all variables and key words used in the specifications. The following fields are presented for each variable:

(1) Short Name: Every variable has a short name that may be used as the data flow name. This entry appears first and is used for alphabetical ordering of the data dictionary.

(2) Qualifiers: Mnemonic representation of the parameters used for subscripting the variable. They follow the short name and may be set off by separators such as parentheses "(" and ")" or hyphens "-" or underscores "_". These qualifiers have data dictionary entries of their own.

(3) Long Name: Every variable also has a long, more explanatory, name consisting of several words, which may be abbreviated, to be used where possible in references to the variable to improve readability, such as in the minispecs.

(4) Definition: Each variable is defined completely in a few sentences that explain what physical quantity the variable represents.

(5) SI units: Metric units are provided for every variable. They appear inside square brackets (e.g. $[mol \cdot a^{-1}]$). Where no units apply, "[-]" is used. Either a solidus "/" or negative exponents may be used to indicate division. There may be, in addition, a field for a "limited character set" representation of the units that can be used when only upper case characters are available.

(6) Sampled/Calculated: The data dictionary states whether a variable is an input (sampled) parameter or a calculated parameter.

(7) Mathematical Symbol: The mathematical symbol used to represent the variable in any supporting documentation, and in the mini-specs, is given together with any qualifiers or indices.

(8) Composition: If an entry is a composite data flow or a data store, representing a collection of other simpler data flows, the composition is indicated. Symbols used to describe the composition are:

= composition, as in A = B, "A is composed of B"

+ concatenation, as in A = B + C, "A is composed of B and C"

[|] alternatives, as in A = [B | C], "A is composed of B or C"

() optional, as in A = B + C + (D), "A is composed of B and C and may optionally include D"

"" explanatory comments are enclosed by quotation marks.

3. CONVENTIONS USED IN GEOSPHERE MODEL SPECIFICATIONS

3.1 ASSUMPTIONS

In the data flow diagrams (DFDs) and data dependency diagrams (DDDs) or minispecs that follow, the system is assumed to be simulated for time $t \geq 0$, one nuclide at a time. When radioactive decay chains are simulated, the nuclides are modelled such that chain precursors are done first. It is assumed that at any location the current time variable, the time of the end of the simulation, t_{sim}, the number and identity of the current nuclide, and the number and identity of radioactive decay chain precursors are available.

Nuclide transport in the geosphere model is calculated from node to node of a network of geosphere transport segments. This network is defined by the connectivities of nodes in pairs to form segments. It is assumed that this connectivity information is available during the simulation. It is also assumed that the nodes at the inlets (or sources) of the network, the nodes at the outlets (or exits, or discharges) of the network, and other special sets of nodes can be identified. A comprehensive list of the "connectivity data" is given in Chapter 9 in the data dictionary entry.

3.2 NOTATION

3.2.1 Process Numbers

To save space, process or bubble numbers shown on the DFDs are abbreviated by giving only the last digit of the complete number. The complete bubble number is obtained by appending the number shown in the bubble to the diagram number on which the bubble occurs. For example, the complete process number for the process depicted in bubble numbered "3" on Diagram 2.2.1 is number 2.2.1.3 and the expansion of this process appears on

Diagram 2.2.1.3. A bubble whose expansion at the next lower level is a DDD (minispec) is shown by a double circle.

3.2.2 Data Flows

In these specifications, variables are assigned alphanumeric names. The names of single variables are composed of up to six upper-case characters. In addition a variable may have optional qualifiers or subscripts (see Arrays); these qualifiers are assigned alphanumeric names of up to six lower-case characters each. The complete data flow name used in the specification consists of the variable name and all relevant qualifiers with the hyphenation symbol used as a separator. Hence the data flow "DECAY-nuc" consists of the variable "DECAY", which has subscript "nuc"; i.e., "DECAY" is a vector with one value for each value of the qualifier "nuc" and the data flow consists of all values. Lowercase only characters are also used for composite data flow names and there is no restriction on the length of the name. The symbols "-" or "_" may be used to make long composite data flow names more readable. Each data flow has its own unique arrowed line indicating the origin and destination for the data. Heavy lines represent data flows that are functions of time; light lines represent data flows that are not functions of time.

The superscript "*" on a data flow name indicates that the data flow appears more than once on the same diagram and each occurrence is so indicated.

As described in Chapter 2, data stores may be introduced on the data flow diagrams. The subsequent transfer of data to and from a data store, originally introduced on a higher level diagram, is indicated by showing the data store at the edge of the diagram with only one of its bounding horizontal line segments.

3.2.3 Composite Data Flows

Data flows are often grouped together into composite data flows to keep the DFDs as simple as possible. Composite data flows are given names in all lower case characters and the catenation symbols "_" or "-" may be used to improve readability. A composite data flow is expanded into its components at lower levels; a definition of the composite data flow in terms of all its component data flows is given on the diagram upon which the expansion has occurred. For example, a bubble may require a composite data flow called "group-a" that is composed of parameters PARA, PARB, and PARC and another composite data flow "group-b". The expansion of "group-b" might occur on a different diagram than the expansion of "group-a". Not all components of a composite data flow are necessarily used in all processes into which the composite data flow is directed. In such cases, in the expansion of the composite data flow in terms of its component data flows, a complete expansion is given and the unused components are marked with the superscript "@". Once expanded, data flows are not subsequently collapsed into other composite data flows. A data flow item appears only once, in only one composite data flow, except in Diagram 0 as explained below.

3.2.4 Data Stores

Data store names consist of all upper case characters and the catenation symbols "_" or "-" may be used to improve readability. Data flows leading to or from data stores consisting of all or several of the data items of the data store are unlabelled. If the data flow consists of only one item from the data store, the flow is labelled. A list of the complete contents of the data store is given with each data flow diagram or minispec on which the data store appears. Unused components of the data store are not noted in this list; only the used components appear in the variable table in a minispec.

3.2.5 Arrays

Some data flows consist of ordered lists or arrays of values of a physical quantity, for example, tortuosities for a set of transport segments. The arrays are indexed by using one or more qualifiers or keys. The keys are denoted by short (up to six lower-case characters) mnemonics used in the data flow name and separated by "-" from each other and from the variable name itself, for example SGTORM-seg. The keys for an array are shown with every occurrence of the variable name on the data flow diagrams. The values for the keys are assumed to form part of the data flow. The context of the DFD or DDD usually indicates whether the subscripted data flow consists of only one component of the array, or a set of components of the array, or the complete array. If the context is insufficient to distinguish, an explanatory note is added.

To keep the mathematical notation as clear as possible, the array keys may be omitted from the mathematical symbol for a physical quantity, when the symbol is used in equations and in the model synopsis. When the array keys are included with the symbol, they are denoted by lower-case letter subscripts on the symbol enclosed within brackets "<" and ">" to separate them from any other subscripts that form part of the symbol name. Any superscripts are always part of the symbol name. For example $\tau_{m,<s>}$ denotes the matrix tortuosity, symbol τ_m, for geosphere transport segments subscripted by array key "s".

The data dictionary has a single entry for each array, with the short name having its associated mnemonic keys. The long name, the full definition, and the mathematical symbol refer to a single component of the array. The mathematical symbol is given with the array keys shown.

On data dependency diagrams, even when the complete array enters the diagram, the definition table gives the definition for only one component of the array and the array keys are indicated with the mathematical symbol. However, the equations may omit the array keys on the mathematical symbols when it is clear which components are being referenced.

3.3 DATA FLOW DIAGRAM 0

Diagram 0 is used in the set of specifications for each of the three models: vault, geosphere and biosphere. In order to maintain a separation between the specifications of the three models, data flows (or composite data flows) may be repeated in more than one of the primary input data flows (spvlt, spgeo, and spbio), all shown on Diagram 0. In all other composite data flows in the geosphere model specifications, a data flow item appears in only one composite data flow.

3.4 CONNECTION WITH ASSOCIATED COMPUTER CODE

Whenever possible, the short name for variables used as a data flow name, which consists of up to 6 upper-case alphanumeric characters, should correspond to the variable name used in the code, but this correspondence does not occur for every variable. The lower-case entries that represent composite data flows and the data store names may be used as names of group storage blocks, such as FORTRAN common blocks, in the code. The mnemonic array keys may be used as subscripting variables, which may be loop indices, in the code.

The data dictionary contains many additional entries for variables and keywords over and above those used with these analysis specifications. Some of these additional entries are associated with the code for the geosphere model.

3.5 EQUATION REFERENCING

In the minispecs, the numbered equations [e.g. Eqn. (4)] are referenced back to the model synopsis equation number using the notation "SEqn.", standing for "Synopsis Equation" [e.g. SEqn. (6.13)]. If reference is made to equations from other reference documents the original equation number is also given using the notation "REqn.", standing for "Reference Equation" [e.g. REqn. (6b)] and the full reference for the document is given in the minispec. If there is more than one reference for the equations, a sequence number is added to the notation [e.g. R1Eqn. (12); R2Eqn. (A3)]. The sequence numbers refer to the references in the order in which they appear in the reference section of the minispec. Where there is no explicit equation in a reference document to refer to, either no reference is made or a reference is made to a section number of the model synopsis or a reference document where the equation is described.

3.6 SUMMARY OF SUPERSCRIPTS

- * Data flow name appears more than once on this diagram. Each occurrence is so indicated.
- e Data flow enters this diagram as part of a composite data flow but is not used on this diagram.