UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D.C. 20555-0001

August 26, 1997

TO: Michael J. Bell, Chief
Performance Assessment and High-Level Waste
Integration Branch, DWM

FROM: James R. Firth JRF
Performance Assessment and High-level Waste
Integration Branch, DWM

SUBJECT: TRIP REPORT FOR DOE WORKSHOP ON VERSION 5.0 OF THE REPOSITORY INTEGRATION PROGRAM (RIP) -- JULY 9-10, 1997

I observed the U.S. Department of Energy (DOE) workshop on RIP, a performance assessment code developed by Golder Associates. This workshop was held to provide DOE contractors with an introduction to the features, capabilities, and use of RIP. The meeting was planned in conjunction with the release of RIP version 5.0. A representative of Sanford, Cohen, and Associates, a contractor for the U.S. Environmental Protection Agency for the Yucca Mountain rulemaking, also observed the workshop.

The meeting began with an introduction into the history and basic philosophy of RIP. This was followed with an overview of the RIP architecture and an example problem. Finally, the important components of RIP were discussed individually. Copies of the tentative agenda and the handouts are attached.

RIP is currently configured with pre- and post-processors that will run on a PC (Windows-95 or Windows NT) and computational routines written in C that can be run on a PC or UNIX workstation. Version 5.0 represents a major upgrade; funding for this upgrade was, primarily, by Golder Associates. RIP complies with NQA-1 and ISO-9001 requirements and has been benchmarked against the Sandia National Laboratories total system performance assessment codes. I have requested a copy of the verification plan used for RIP.

DOE is using RIP in its performance assessments for Yucca Mountain. The current version of RIP allows external program modules to be linked to RIP using dynamic link libraries (DLL's); linking requires the user to develop a shell around the external program to allow the program to be called by RIP without modifying RIP. There is an effort underway to run Finite Element Heat and Mass Transfer Code (FEHM) as an external module to perform the transport calculations. Also, Intera is working on incorporating colloidal transport models into the DOE RIP model for Yucca Mountain.

The current DOE philosophy for modeling the engineered barrier system includes consideration of the following: waste form, cladding, waste package, corrosion products, and invert, using 4-5 major components in the model.

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Also, DOE is considering whether to divide the repository into two areas -- center and edge, defined by temperature and water flux. Further, because climate change cannot be included within a realization, DOE will try to address this issue using bounding estimates.

DOE is considering its quality assurance needs for using RIP. They plan on using some of their experience acquired from using RIP for the Waste Isolation Pilot Plant (WIPP). Currently, there is no way to confirm the pedigree of external programs used within RIP. A failure to adequately address this issue could lead to reproduceability and QA concerns.

There are several aspects of RIP that are of potential concern:

- RIP allows physically unrealistic calculations.
- RIP does not balance mass of storage or transport media.
- RIP will calculate diffusive particulate releases from cell pathways into pipe pathways; however, pipe pathways will only transport dissolved material.
- RIP uses explicit solution routines, which may require short time steps for some applications to retain accuracy; RIP will not calculate iterative solutions.
- There are potential problems with the use of pipe transport pathways within RIP:
  - (e.g., numerical artifacts and sensitivity of dose calculations to modeling of breakthrough curves);the presence of user specified breakthrough curves will require examination of supporting calculations to confirm their appropriateness.
  - Retarded radionuclides may be released from pipes very slowly (non-conservatively) when they enter the pipe with less retarded radionuclides.
  - Daughter products are released from the pipe at the same rate as the parent.
- RIP may not conserve mass if external flow paths are defined.

Attachments: 1. Tentative Agenda
2. Workshop Handouts

DISTRIBUTION: Central File, PAHL r/f, EBrummett, JThoma, NEisenberg, TRothschild, TMcCartin, RBacca/CNWRA

DOCUMENT NAME: S:\DWM\PAHL\JRF\RIPTRIP.RPT

| OFC | PAHL | | PAHL | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| NAME | JFirth/kv JRF | | KMcConnell | | | | | | | |
| DATE | 8/27/97 | | 8/26/97 | | | | | | | |

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# Tentative Agenda

RIP WORKSHOP
July 9-10, 1997
Las Vegas

**Wednesday, July 9**

| | |
|---|---|
| 1:00 - 3:00 | Introduction<br>RIP Philosophy and Approach<br>RIP Overview |
| 3:00 - 3:15 | Break |
| 3:15 - 5:15 | Simple Example<br>The RIP Parameters Module |

**Thursday, July 10**

| | |
|---|---|
| 8:00 - 10:00 | Transport Pathways |
| 10:00 - 10:15 | Break |
| 10:00 - 12:00 | Source Term<br>Representing Spatial Variability |
| 12:00 - 1:00 | Lunch |
| 1:00 - 3:00 | Receptors<br>Disruptive Events<br>Post-Processsing |
| 3:00 - 3:15 | Break |
| 3:15 - 5:00 | Sampling Details<br>General Discussion |

Attachment 1

Wrd with letter dtd 8/26/97
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# RIP

## An Integrated Probabilistic Simulator for Environmental Systems

***A child of five would understand this. Send someone to fetch a child of five.***

**Groucho Marx**



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Attachment 2

# Workshop Objectives

- **Provide introduction to the features, capabilities and use of RIP**
- **By the end of the workshop:**
  - You will have a good understanding on what RIP is, and how it can be applied
  - Depending on your experience in PA, you may be able to create, run and evaluate simple RIP applications
  - Advanced applications will require:
    - **additional training**
    - **detailed reading of the RIP Theory Manual and User's Guide**
    - **practice**



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# Outline

- **What is RIP?**
- **RIP Philosophy and Approach**
- **Overview of RIP Component Models**
- **Software Structure and Introduction to User Interface**
- **Applying RIP**
  - The RIP Parameters Module
  - Transport Pathways
  - Source Term
  - Representing Spatial Variability
  - Receptors
  - Disruptive Events
  - Post-Processing Results
  - Sampling Details



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# What is RIP?

- PC-based software program which probabilistically simulates the release, transport and fate of contaminants in complex engineered and/or natural environmental systems
- RIP is a "total system" model intended to integrate all key aspects of complex systems



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# Key Features of RIP

- Top-Down design allows arbitrary level of detail: Extreme flexibility of the tool allows component models to be very simple or very complex
- Allows user to explicitly represent both uncertainty and variability in system parameters
- Integrates four component models: Source Term, Geosphere, Biosphere, and Disruptive Events

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# What Can RIP Do?

- Integrate all aspects of a complex environmental system
- Predict the long-term performance of the system (in terms of contaminant releases, concentrations, and doses)
- Assess the sensitivity of system performance to individual parameters and processes

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# RIP Computational Features

- Easy-to-Use interface, with graphical capabilities
- Pre-processor and Post-Processor run on personal computers
- Computational routines written in C: can be run on nearly any machine
- On-line context sensitive help screens

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# RIP History

- Development started in 1990 at the request of DOE OCRWM to support Yucca Mountain
- Continued development through Version 4 funded internally and by numerous clients worldwide
- Version 5 represents major upgrade
  - funded primarily internally
- Total RIP development effort estimated at approximately 15 man-years



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# Some Major RIP Applications

- Yucca Mountain
- WIPP
- ENRESA (Spanish HLW program)
- New York LLW
- Illinois LLW
- Hungary LLW
- Dounreay Disposal Shaft (Scotland)
- WISMUT Uranium Mill Tailings (Germany)
- Ph.D. Theses (Iowa State)



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# Documentation, Configuration Management and Verification

- Detailed Theory Manual and User's Guide
- Suite of approximately 500 verification tests included in Verification Report
- Automated configuration management and bug-tracking system
- Complies with NQA-1 and ISO-9001 requirements
- Benchmarked against independent total system codes developed by Sandia



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# Purpose of Performance Assessment

- Organize and integrate the large amount of steadily evolving information required to design and license a disposal facility or remediation plan
- Guide decision-making throughout the design, site-selection, site characterization, and engineering process
- Establish a safety case



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# Golder's Performance Assessment Philosophy

- Performance assessments should be iterative, flexibly evolving with time as more information is obtained
- Performance assessments should be based on a "Top Down" conceptual model of system behavior
- Uncertainty in the system should be explicitly represented in order to predict uncertainty in results and/or facilitate sensitivity/uncertainty analyses



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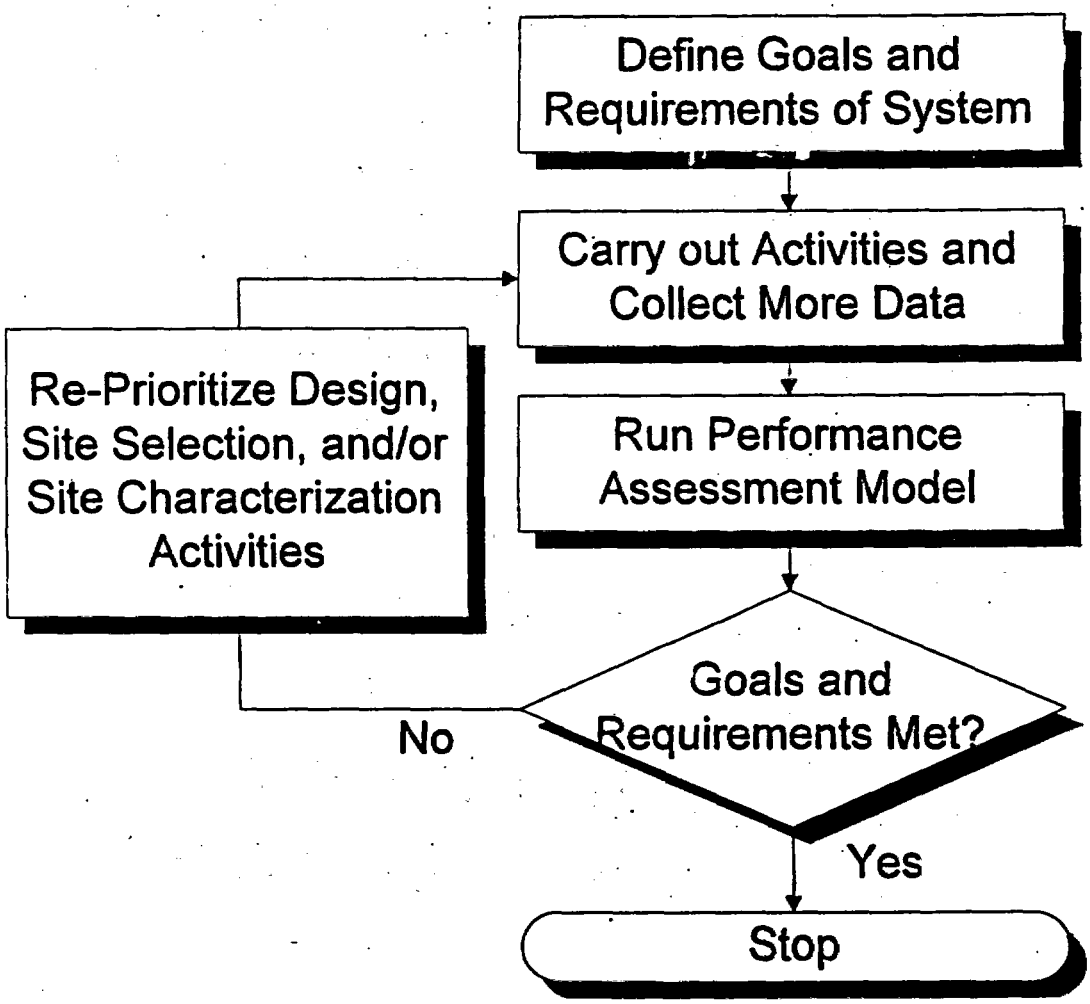
# Iterative Performance Assessment

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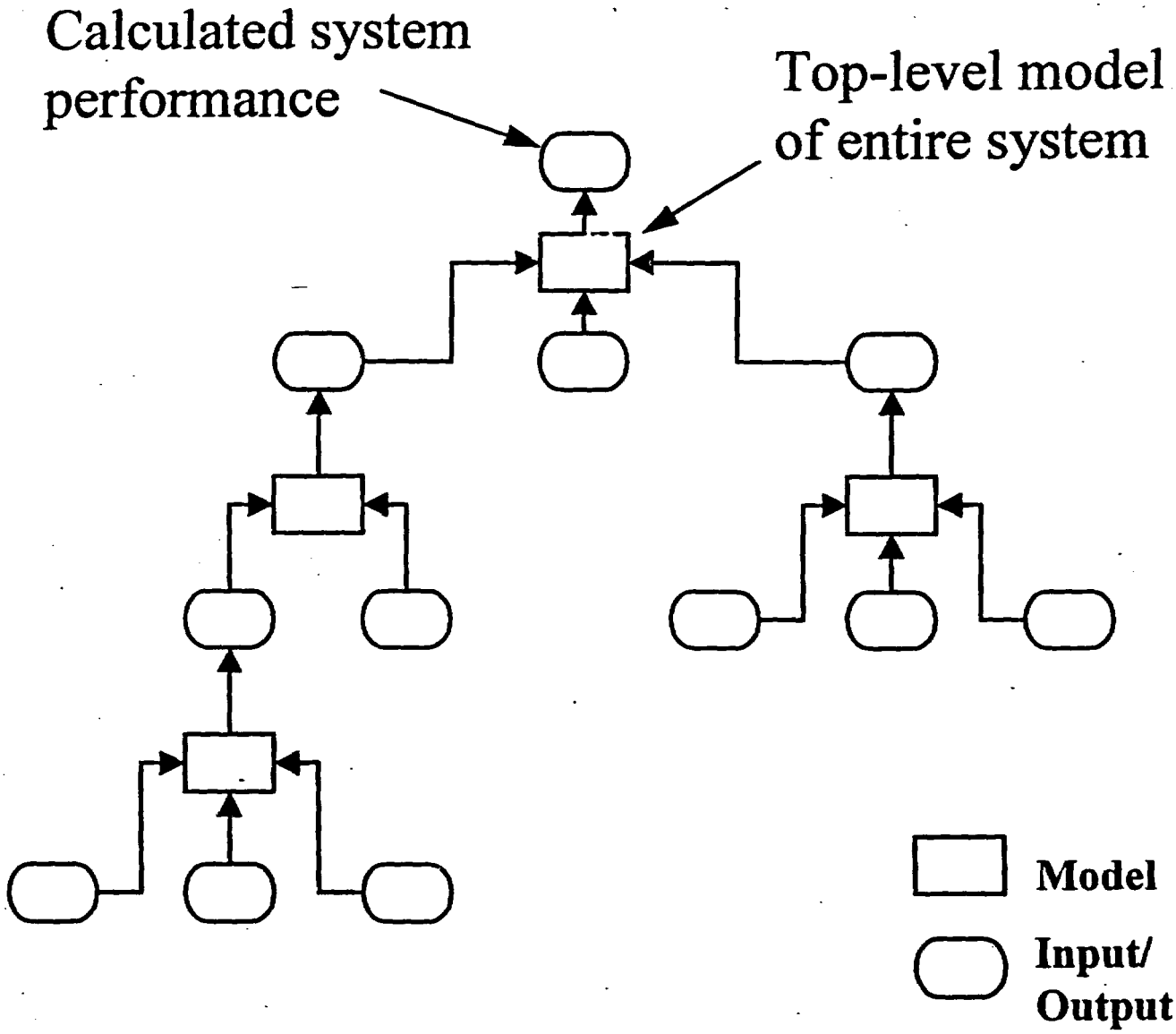
# Performance Assessment Approaches

- **"Bottom-Up" Approach**
  - program is driven by scientists and engineers studying various aspects of the system
  - typically not well integrated with a poorly defined endpoint
- **"Top Down" Approach**
  - attempts to integrate performance of entire coupled system at a high level
  - details added as required
  - goals and endpoint are well defined

# Top-Down Approach to Performance Assessment

- Concentrates on developing a consistent framework for integration (coupling) of all components of the system
- Focuses on performance, not on process
- A properly designed top-down model is not "simple"; it strives to approximate the impact of all key features and processes
- This approach helps keep projects focused without spending time and money on irrelevant matters

# Top-Down Structure



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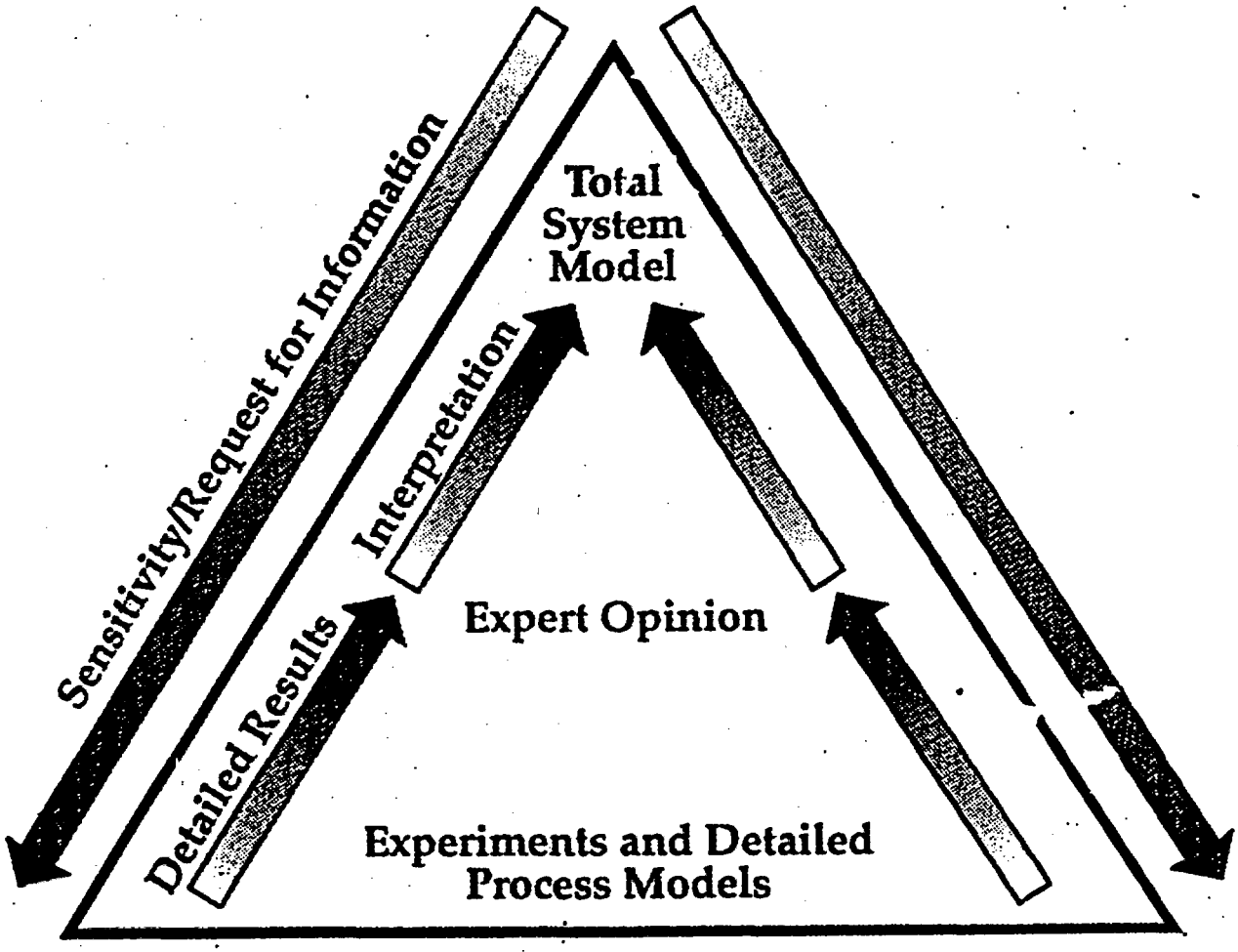
# "Top Down" Performance Assessment Structure



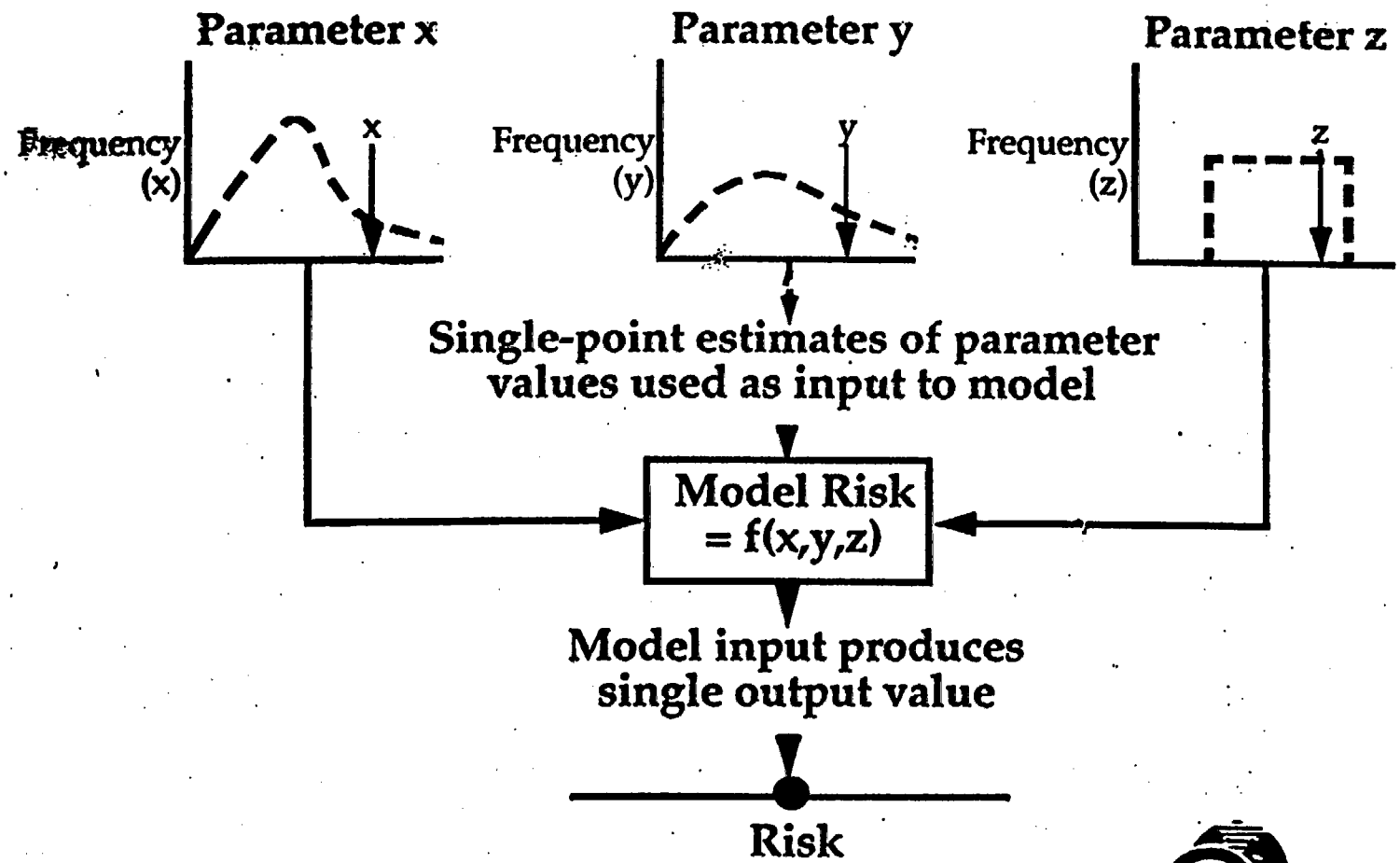

IC3 1032

# Deterministic and Probabilistic Approaches to PA

- **Deterministic**
  - use "best estimate" or "worst case" parameter values
  - individual component models are typically more detailed
- **Probabilistic**
  - use probability distributions to represent model parameters
  - individual component models typically less detailed (due to computational considerations)
  - directly facilitates sensitivity and uncertainty analyses

# Deterministic Model Structure

*Possible range for each input parameter determined*



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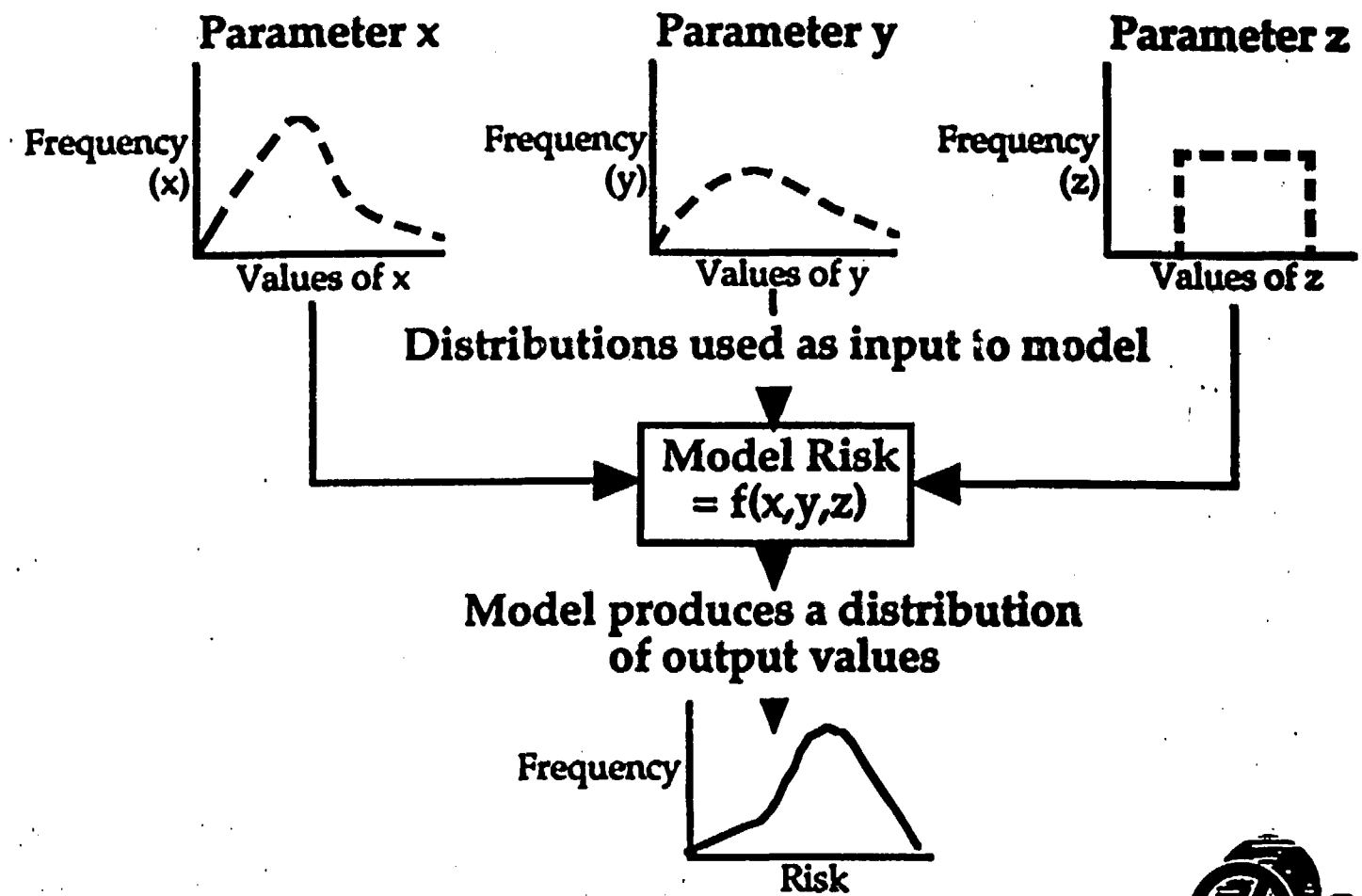
# Probabilistic Modeling Approach

*Distributions Estimated for Each Parameter*



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# Deterministic vs. Probabilistic (cont.)

- **Deterministic PA is likely to encounter difficulties**
  - What does "worst case" represent?
  - Any facility can be made to fail for a given set of "worst case" parameters
- **Key points:**
  - It will never be possible to claim with absolute certainty that a facility will meet performance criteria
  - Performance predictions can only presented in terms of the likelihood of meeting criteria
  - Probabilistic PA provides a means to quantify this likelihood in a defensible way

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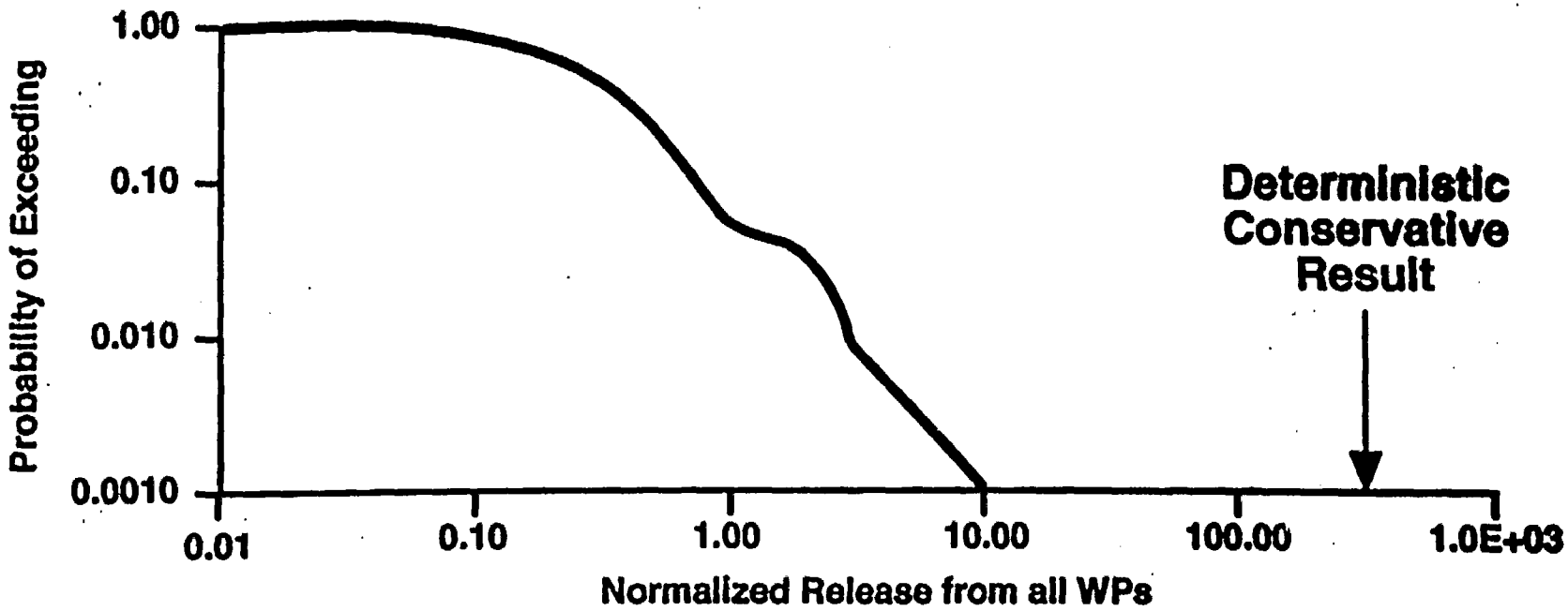
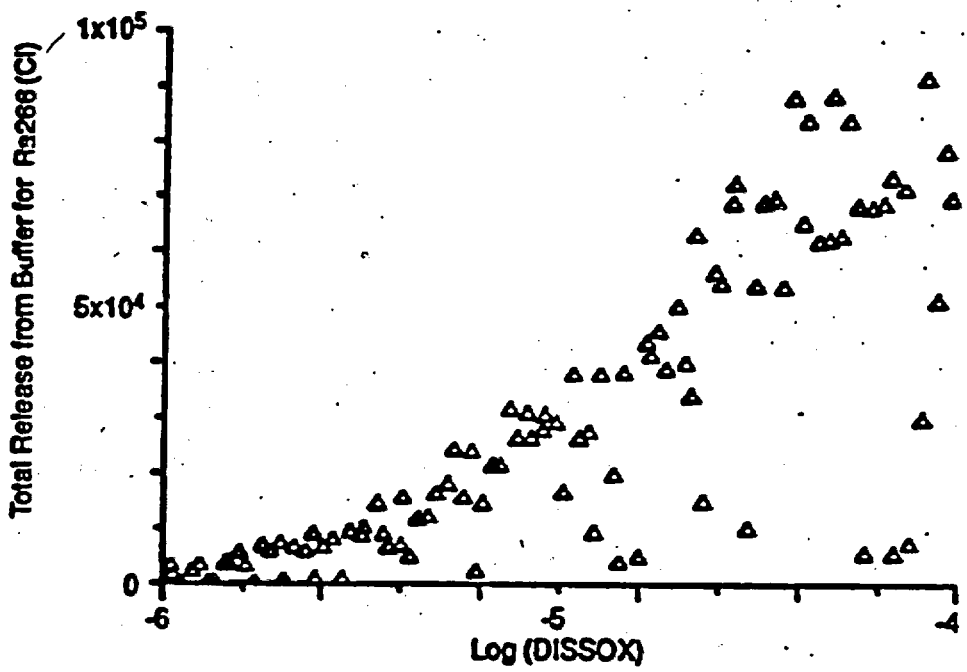
# Waste Package Release






| Dwg. 004 | Rev. 0 | Date: 05-10-92 | Project No. IC31032 | Drawn by: TK |
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Figure 8.4: Ra-226 Cumulative Release as a Function of Matrix Dissolution Rate

# In order to reflect this philosophy and approach, RIP was designed around the following key features:

- Flexibility: Readily describe the system at whatever level of detail is required.
- Ease of Use: Quickly modify the system to permit practical iterative analysis.
- Direct Representation of Uncertainty: Describe inputs as probability distributions.

# RIP Component Models

- RIP simply provides a framework for building a representation of the system
- Similar to a spreadsheet: complexity of the model is determined by the user
- While incorporating some basic physics (e.g., decay and ingrowth), very few assumptions built into code in order to maximize flexibility

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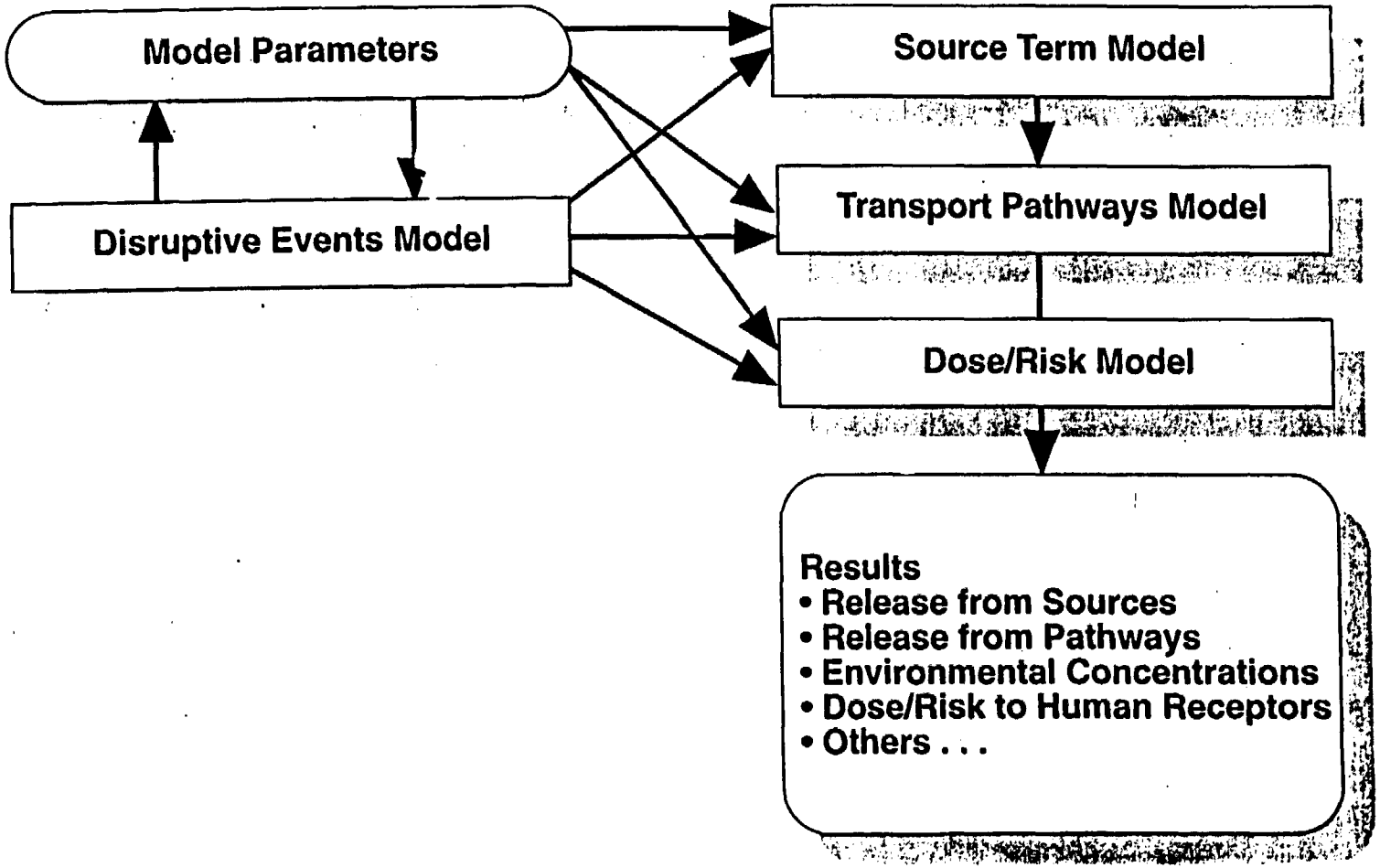
# RIP Component Model Structure



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# Introducing Mass Into RIP

- Specify an initial condition or boundary condition at various locations within Transport Pathways Model
- Define the properties of one or more sources, and simulate the resulting release rates using the Source Term Model



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# RIP Source Term Model

- **Couples the following processes:**
  - failure of any engineered barriers (e.g., corrosion of drums, containers)
  - dissolution of waste form
  - solubility limitations and sorption within waste form
  - advective and diffusive release mechanisms
- **Linked directly to geosphere model**

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# RIP Transport Pathways Model

- Simulates the transport and fate of contaminants in the system
- Based on network of transport pathways
- A transport pathway is function (an operator) whose input is a mass flux and output is a mass flux
- Three types of pathways:
  - cells
  - pipes
  - external pathways



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a) Transport Pathway

b) Network of Transport Pathways

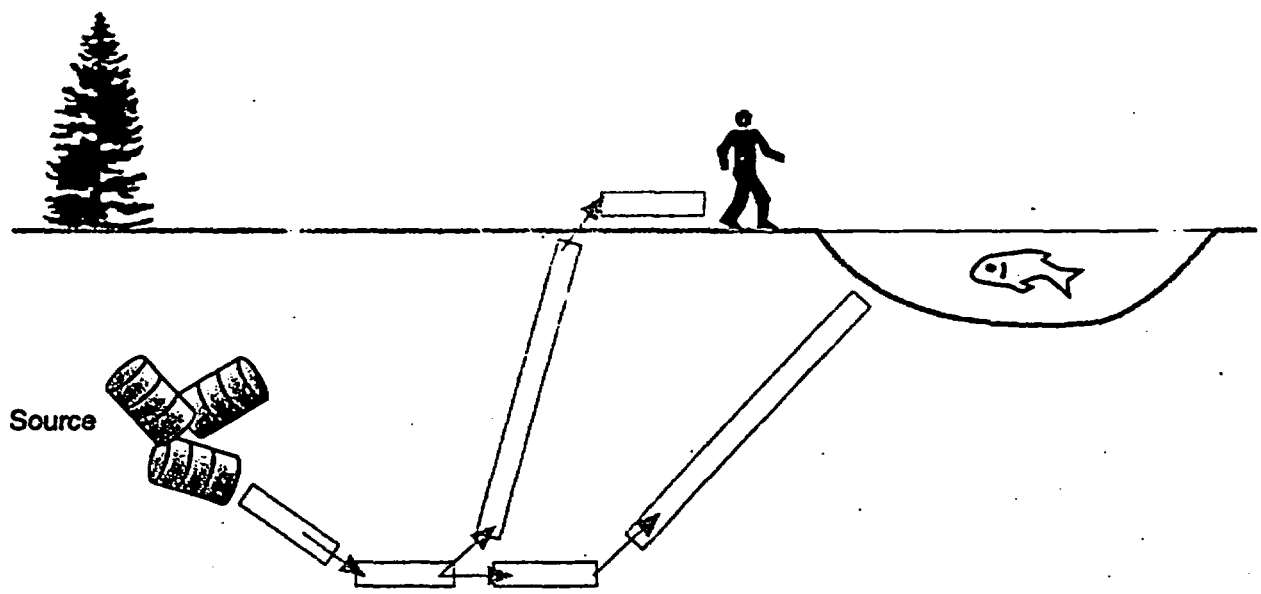


FIGURE 9-1
TRANSPORT PATHWAYS SCHEMATIC

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# Cell Pathways

- One or more fluid or solid media must be assigned to each cell
- For each fluid medium, can also specify particulates that are suspended in the fluid
- All contaminant mass is assumed to be instantaneously and completely mixed throughout the cell
- Contaminant species are assumed to be at equilibrium with respect to partitioning among the various cell media
- Solubility limits are imposed

# Pipe Pathways

- Intended to represent pathways which behave as fluid conduits.
- Mass is transported based in user-specified breakthrough curve.
- Complex breakthrough curves can be simulated by defining multiple flow modes.
- Very computationally efficient way to transport mass through conduits.

# External Pathways

- Provides mechanism by which external program modules for contaminant transport can be linked into RIP (as DLLs).
- User defines inputs and outputs to external pathways: RIP passes information back and forth in appropriate manner.

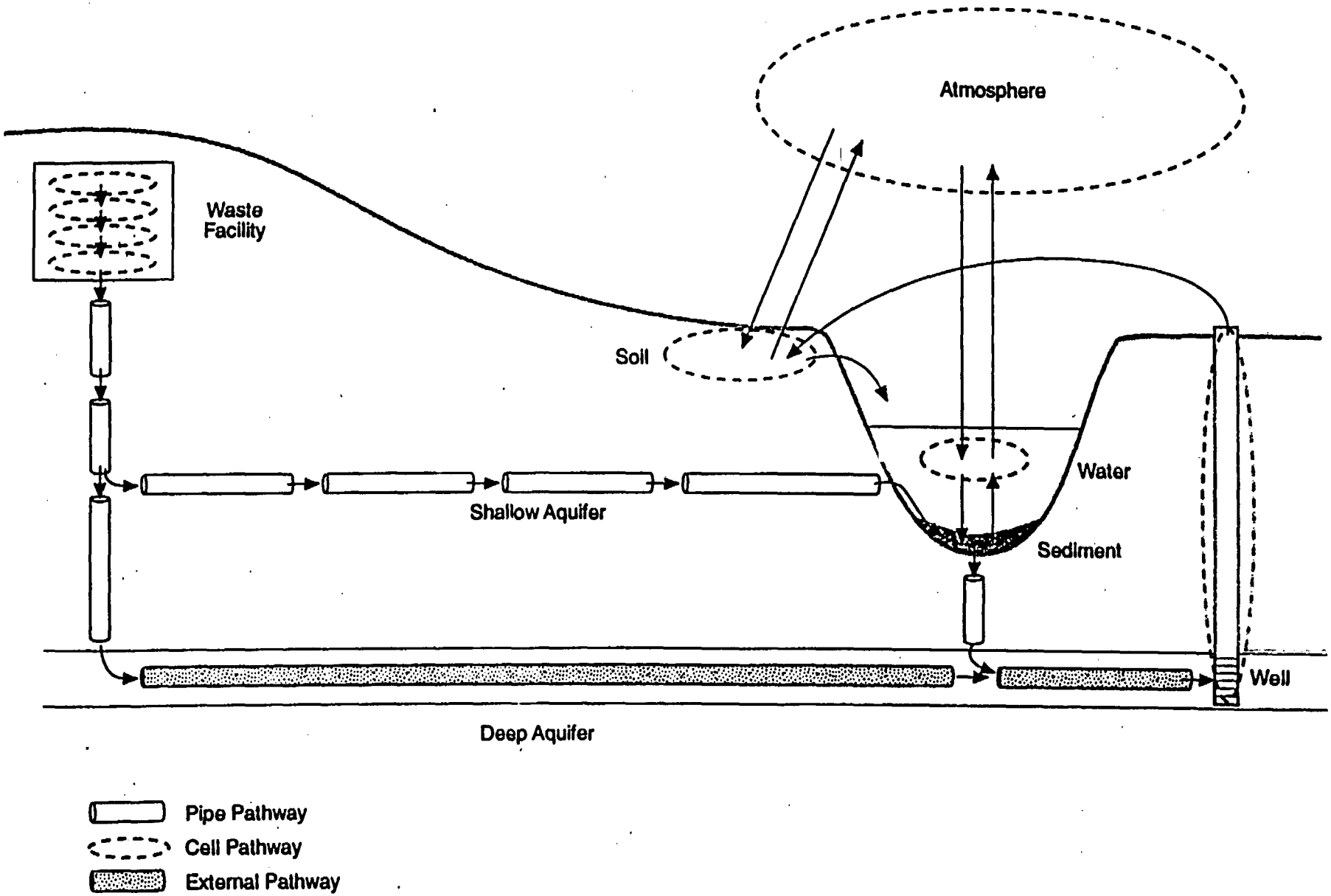


FIGURE 9-2
PATHWAY NETWORK

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# RIP Biosphere Model

- **Converts concentrations in various media to doses to human receptors**
  - Simulates radionuclide transport through the biosphere (e.g., plants, soil, biota) through use of mixing cells and transfer factors
  - Simulates human exposure and uptake of contaminants (e.g., ingestion, inhalation, immersion)

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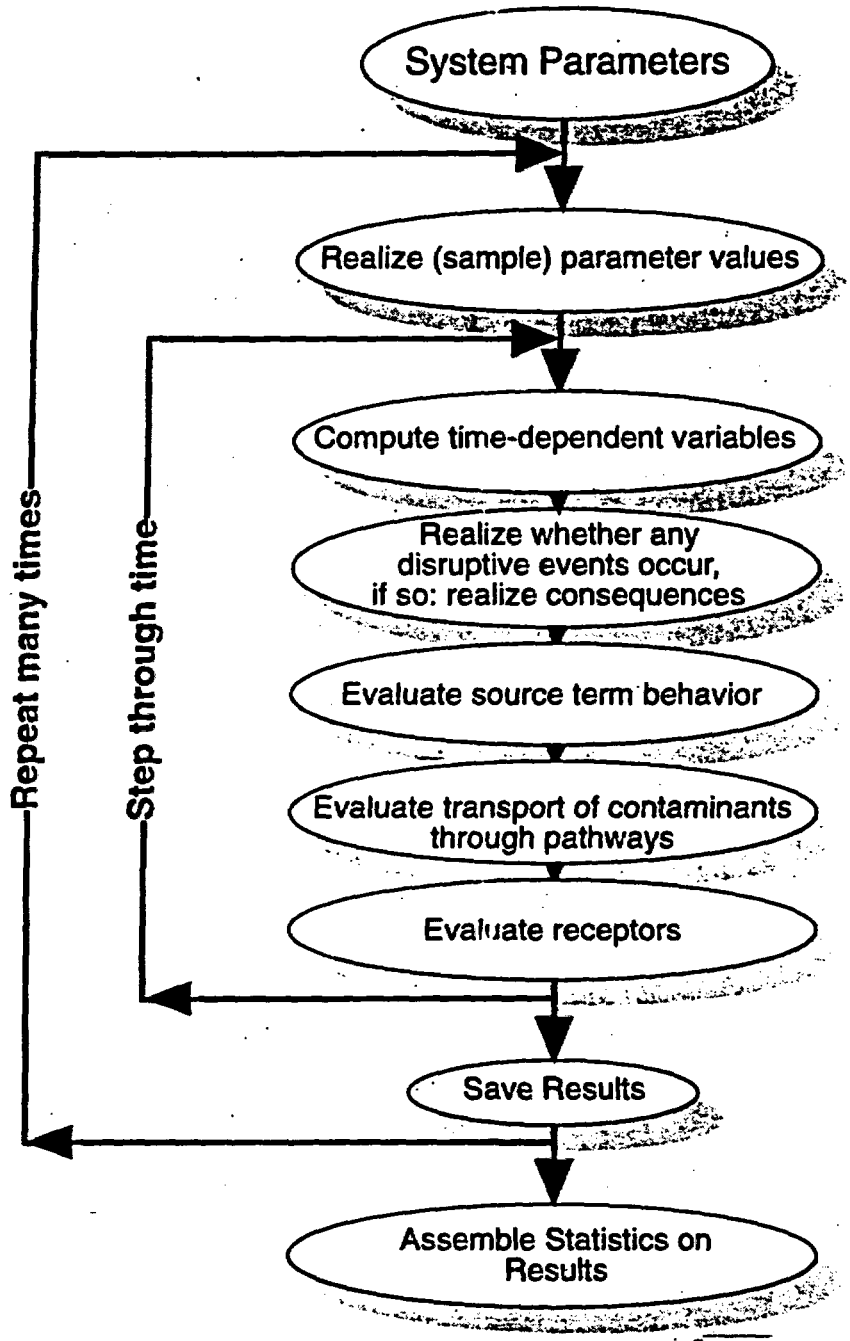
# Disruptive Events Model

- Allows events such as earthquakes, volcanism, and human intrusion to be represented
- Events can occur at regular intervals, when a certain condition is met, or as Poisson processes
- An event can have consequences on the other component models:
  - move mass
  - fail containers
  - modify parameters

# RIP Simulation Logic



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# Propagation of Uncertainty

- **RIP uses the Monte Carlo method to propagate uncertainty**
- **Latin-Hypercube sampling can be specified**
- **Enhanced sampling methods:**
  - biased sampling of parameter tails
  - biased sampling of events

# RIP Outputs and Post-Processing Capabilities

- **RIP Outputs**
  - Impacts (doses and/or health risks) to receptors
  - Release rates from specified sources and or pathways
  - Concentrations in environmental media in specified pathways
- **Built-in post-processing capabilities:**
  - result screening
  - statistical and graphical analysis:
    - **distributions**
    - **time history plots**
    - **scatter plots**
    - **correlation analysis**
    - **file export**



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Results of 100 Monte Carlo realizations.
Mean= 44.18048
S.D.= 7.125189

FIGURE 3-9
CUMULATIVE DISTRIBUTION FUNCTION OF A [illegible]

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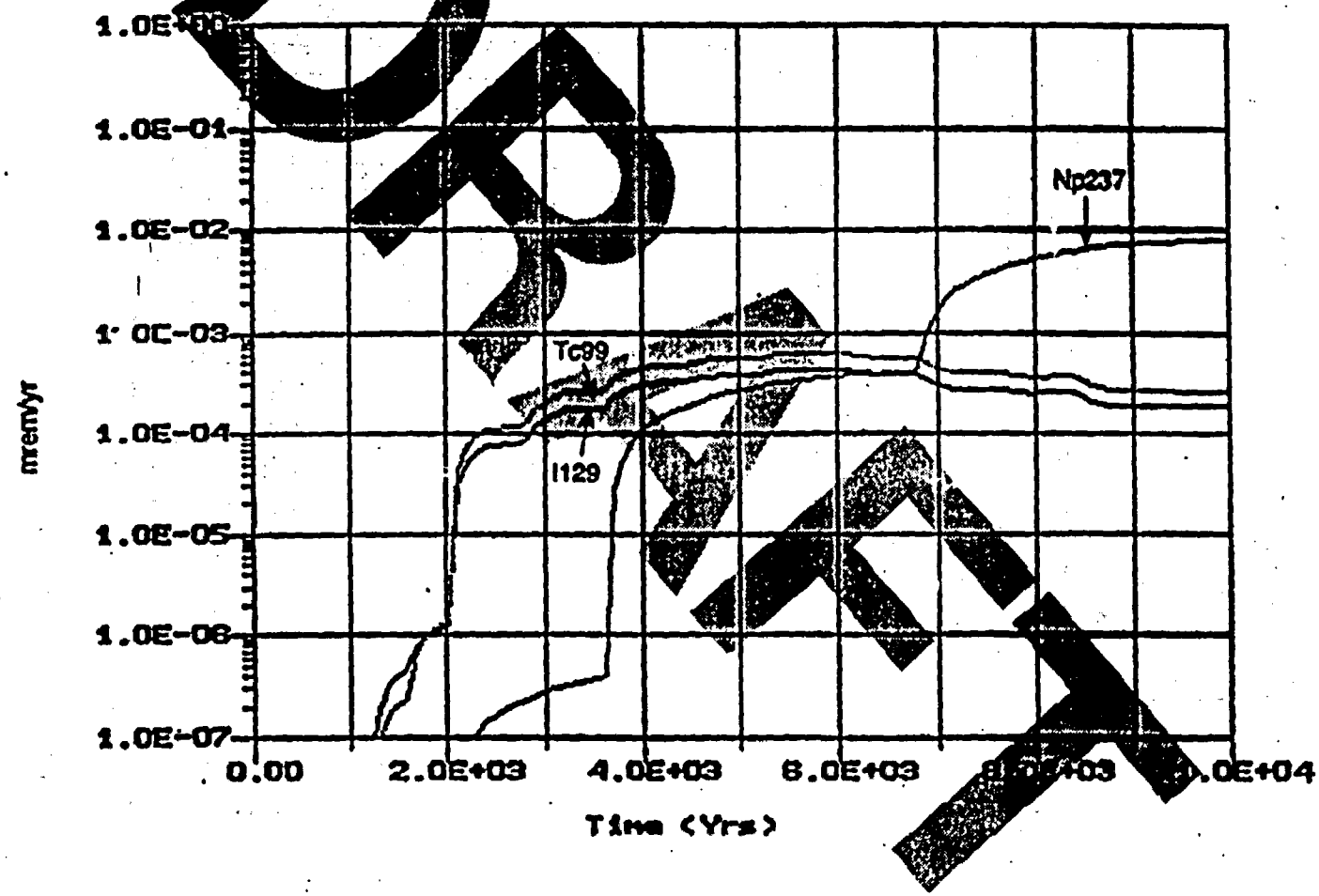


FIGURE 4-3
TIME HISTORY OF DOSE
(10,000 YR SIMULATION USING
EXPECTED VALUES)
EPRI/HLW RAPOS/WA

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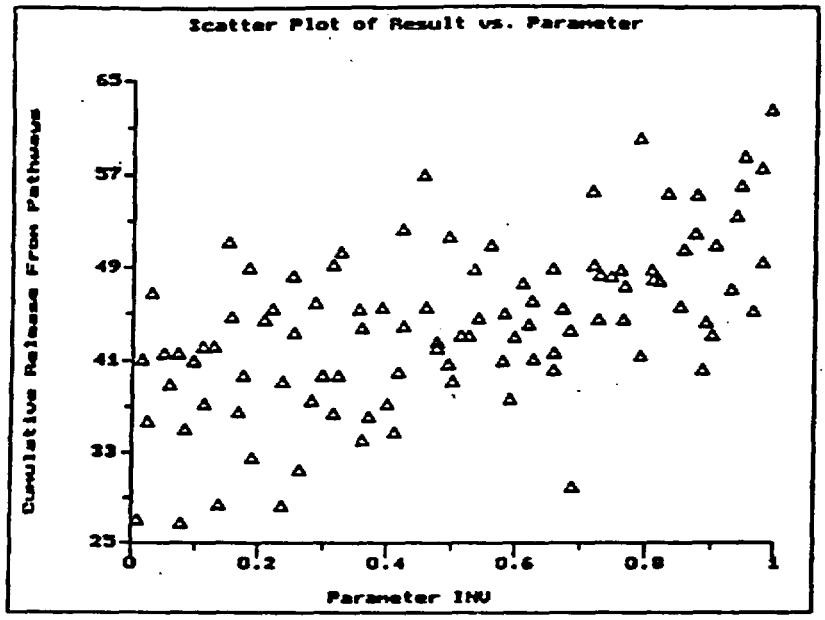
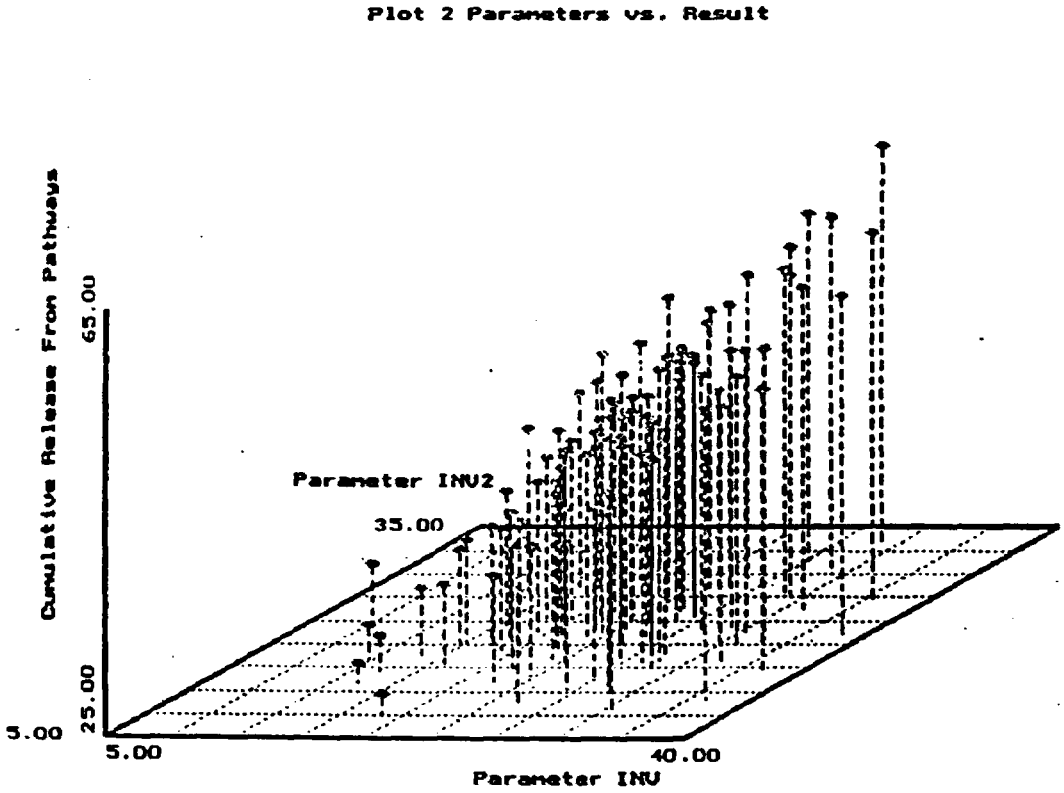



a) One-Dimensional




b) Two-Dimensional

FIGURE **3-11**
**SCATTER PLOT OF RESULTS**

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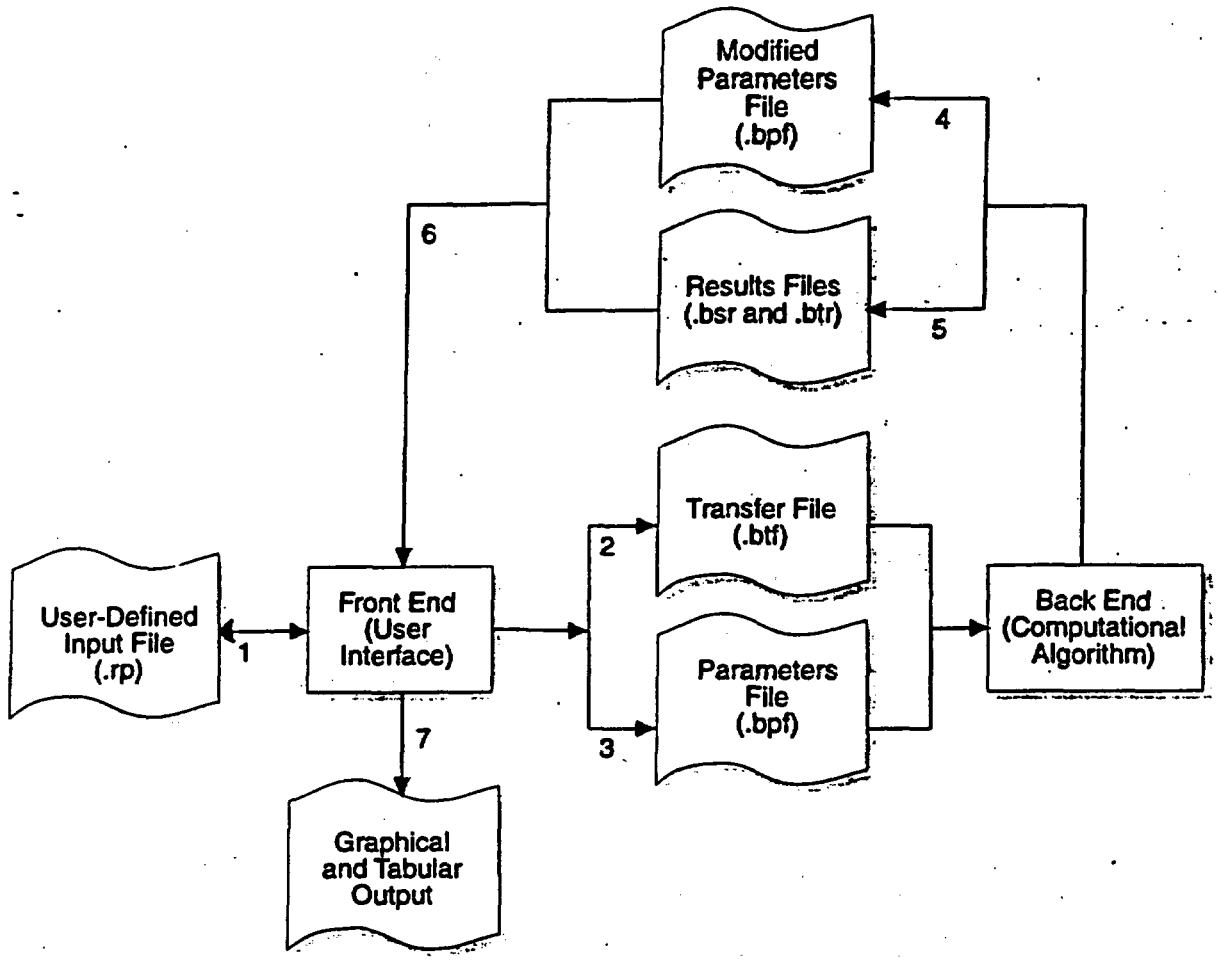


1. Read and/or create input data set.
2. Create transfer file.
3. Write realized values of stochastic, event and constant parameters.
4. Update binary parameters file (dependent parameters).
5. Run back end and produce results.
6. Read results into front end for post-processing.
7. Post-process results.

FIGURE **4-1**
**RIP FRONT END/BACK END STRUCTURE**

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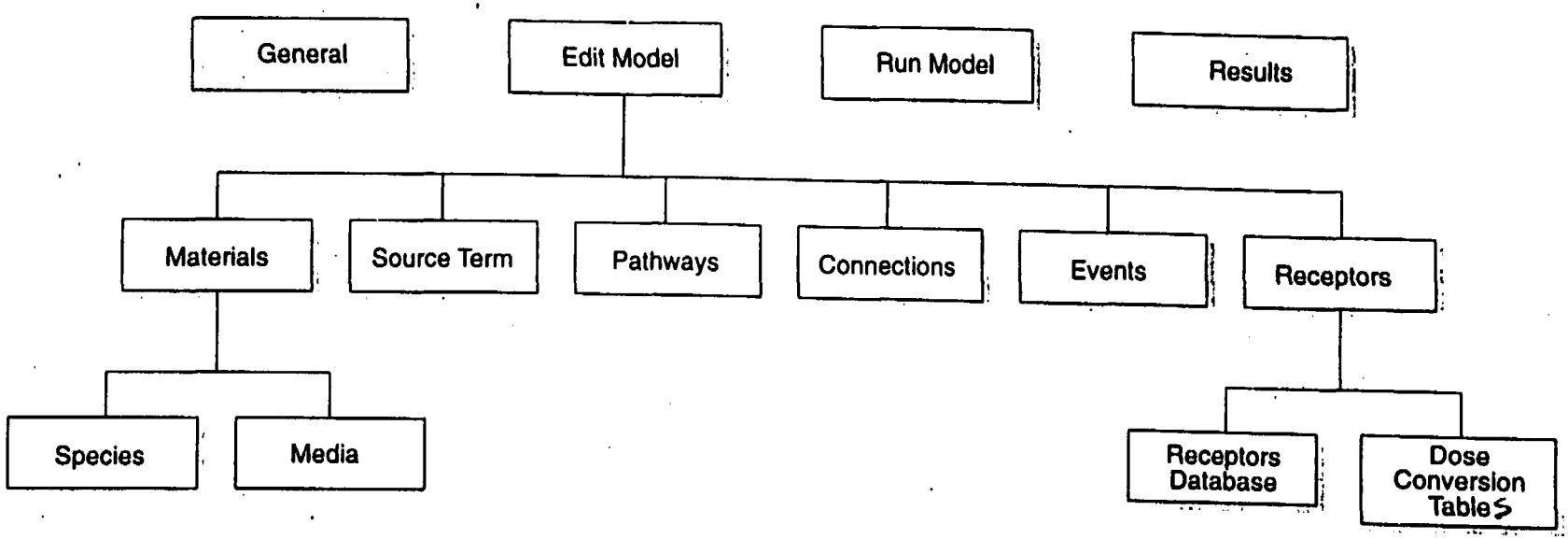


FIGURE 5-1
RIP MENU STRUCTURE

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# Building a System in RIP

- Define Materials
  - species and media
- Define Pathways
- Define Connections
- Define Sources
- Define Receptors
- Define Events
- Create transfer file
- Run back end
- Post-Process results



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# RIP Parameter Module

- **Most important component of the RIP computer code: the cornerstone of the entire methodology**
- **Imparts tremendous flexibility by allowing model parameters to be defined as:**
  - constants
  - probability distributions
  - functions of other defined parameters
  - look-up tables

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# RIP Parameter Types

- constant
- stochastic
- function
- table
- time-integral
- event
- external
- variable

# Stochastic Parameters

- **Wide variety of distributions can easily be input by the user**
  - normal, log-normal, uniform, log-uniform, triangular, log-triangular, beta, gamma, Weibull, Poisson, binomial, Boolean, discrete, cumulative
- **The parameters describing these distributions can themselves be constants, stochastics, or functions**

# Analytical Function Parameters

- **standard mathematical operators**
  - +, -, /, *, **, ()
- **standard relational operators**
  - =, >,<,<=, >=, AND, OR, NOT, NE
- **Special functions**
  - sin, cos, tan, cot, asin, acos, atan, sinh, cosh, tanh, erf, log, ln, exp, min, max, Bess, beta, sqrt, abs
- **IF, THEN logic**

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# Numerical Function Parameters

- If a parameter cannot be represented analytically, user can write a C function which can be linked directly into code
- Input arguments are other RIP parameters
- Output arguments become RIP parameters which can be used throughout the model
- User specifies when and how function is called

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# Look-Up Tables

- **Often, detailed process level modelling or experimental results can most easily be expressed as a response surface, rather than an analytical function**
  - e.g., Solubility = f(pH, redox, other parameters)
- **RIP allows the user to define multi-dimensional look-up tables (response surfaces) to define parameters**

# Defining Species

- Can read ASCII file when RIP file is first created OR can enter directly through the interface
- Species names can.be letters and numbers: letters prior to first number define element
- Species can decay to up to two daughter products
- User specified stoichiometry
- Decay rate can be a parameter and can be spatially and temporally variable
- Can identify radioactive species(whose input/output can be specified in terms of activity)

# Environmental Media

- **Two types (fluids and solids)**
- **Requires a reference fluid**
- **Reference fluid requires:**
  - elemental solubilities
  - diffusivities
- **Other fluids require:**
  - element partition coefficients (e.g., Henry's law)
  - diffusivities
- **Solids require:**
  - element partition coefficients (Kd)
  - porous medium properties
  - particulate diffusivities in fluids
- **Media properties can be spatially and temporally variable**



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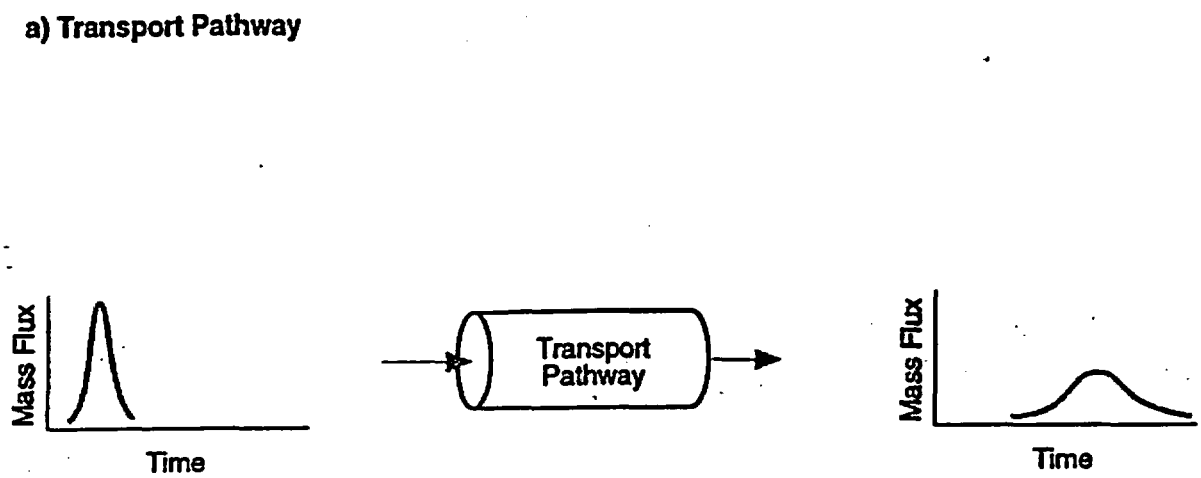


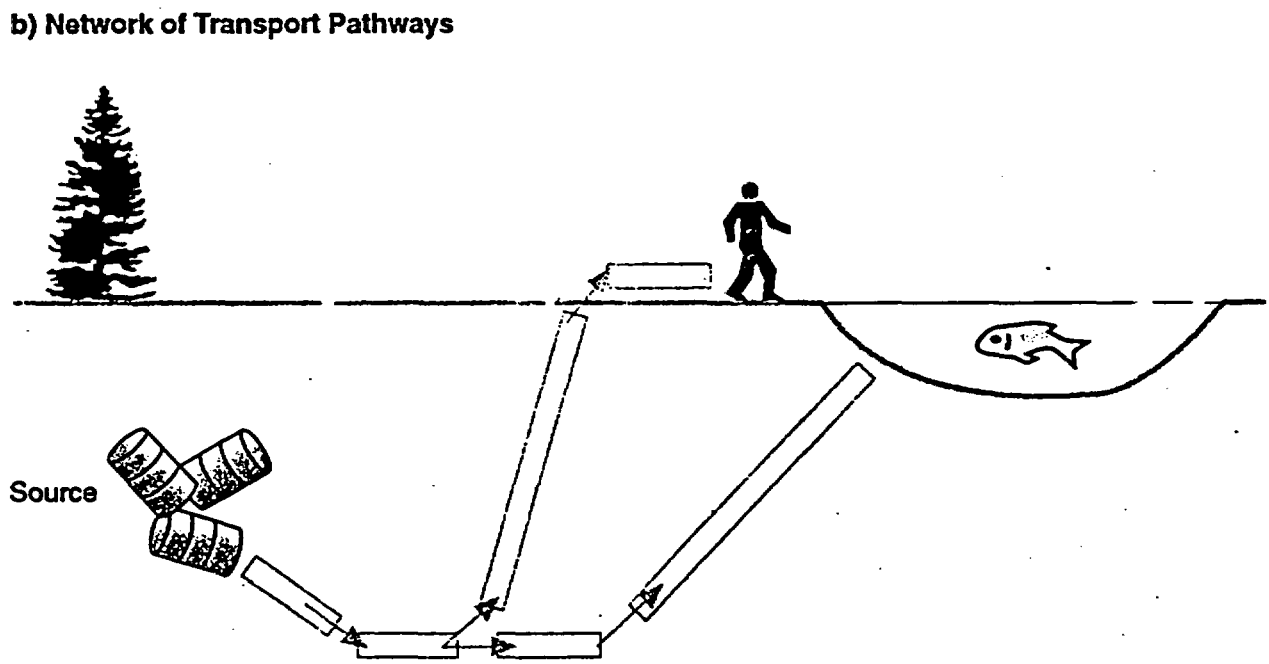


FIGURE 3-4
TRANSPORT PATHWAYS SCHEMATIC

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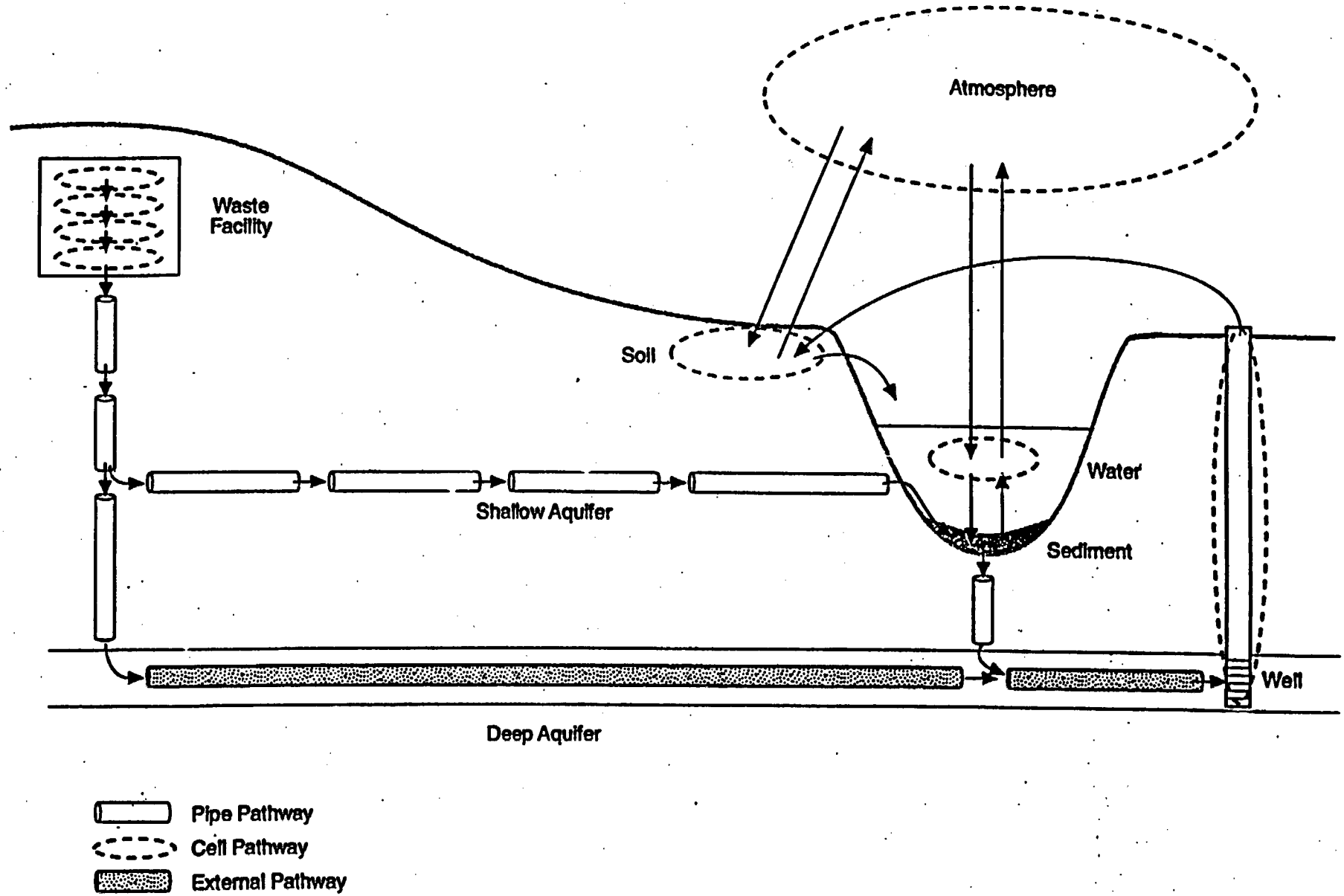


FIGURE 3-7
PATHWAY NETWORK

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# Mass Balance of Media in a Pathway Network

- RIP is a contaminant transport model, NOT a flow model
- RIP does not balance mass of transport and storage media
- User must enforce mass balance on transport media
- RIP will provide non-fatal warning for some flow imbalances
  - flow out < flow in



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# Mass Transfer Connections

- Connect pathways within a pathway network
- Must specify connecting (from) and connected (to) pathways
- Two types:
  - advective
  - diffusive
- Multiple connections can be defined between pathways
- Connections always have two halves

# Advective Connections

- **Depends only on concentration in connecting (from) pathway**
- **Must specify medium flowing**
- **Must specify flow rate**
  - $m^3$/yr for fluids
  - kg/yr for solids
- **Both connected pathways must contain the medium being advected**
- **Only cells can:**
  - be involved in advective connections of solids
  - transport suspended particulates



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# Diffusive Connections

- **Depend on concentrations on both pathways**
- **For both connection halves, must specify:**
  - fluid medium
  - porous medium (if any)
  - diffusive length
- **For entire connection, must specify diffusive area**
- **Connection can involve different fluids (inter-media transport)**
- **For pipes and external pathways, there is no resistance on receiving side of connection (length =0; C =0)**

# Cell Pathways

- Act as mixing cells with multiple media
- Mass is instantly mixed and equilibrated within cell
- Solubility constraints can be imposed
- Behavior of cell network is mathematically equivalent to network of finite difference nodes
- Can have specified initial and boundary conditions

# Conservation of Mass in Cell

$$= S_{is} - m_{is}\lambda_s +$$

$$m'_{is} = S_{is} - m_{is}\lambda_s + \sum_{p=1}^{NP_s} m_{ip}\lambda_p f_{ps} R_{sp}(A_s / A_p) + \sum_{c=1}^{NC_i} f_{cs}$$

$S_{is}$ = rate of direct input of species s to cell i from a source term or an external source [M/t];

$m_{is}$ = mass of species s in cell i [M];

$\lambda_s$ = decay rate for species s [1/t];

$f_{ps}$ = fraction of parent p which decays into species s

$NP_s$ = number of direct parents for species s;

$R_{sp}$ = stoichiometric ratio of moles of species s produced per mole of species p decayed;

$A_s$ = atomic weight of species s

$A_p$ = atomic weight of species p

$NC_i$ = number of mass transfer connections to cell i; and

$f_{cs}$ = influx rate of species s (into cell i) through connection c [M/t].

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# Advective Connections

$$f_{cs} = -\left(c_{ims} + \sum_{t=1}^{NPT_{im}} PFAct \cdot c_{its} \cdot cp_{imt}\right) q_c$$

| | | |
|---|---|---|
| $q_c$ | = | the rate of advection for connection c; |
| $c_{ims}$ | = | dissolved or sorbed conc. of species s in medium m in cell i; |
| $c_{jns}$ | = | dissolved or sorbed conc. of species s in medium n in cell j; |
| $NPT_{im}$ | = | number of solid media suspended in medium m within cell i; |
| $NPT_{jn}$ | = | number of solid media suspended in medium n within cell j; |
| PFAct | = | flag if advection of solid t suspended in the advecting fluid is allowed for connection c; |
| $c_{its}$ | = | sorbed or precipitated concentration of species s in solid medium t within cell i; |
| $cp_{imt}$ | = | the concentration of solid particulate t within fluid m in cell i; |
| $c_{jts}$ | = | sorbed or precipitated conc. of species s in solid medium t within cell j |
| $cp_{jnt}$ | = | concentration of solid particulate t within fluid n in cell j |

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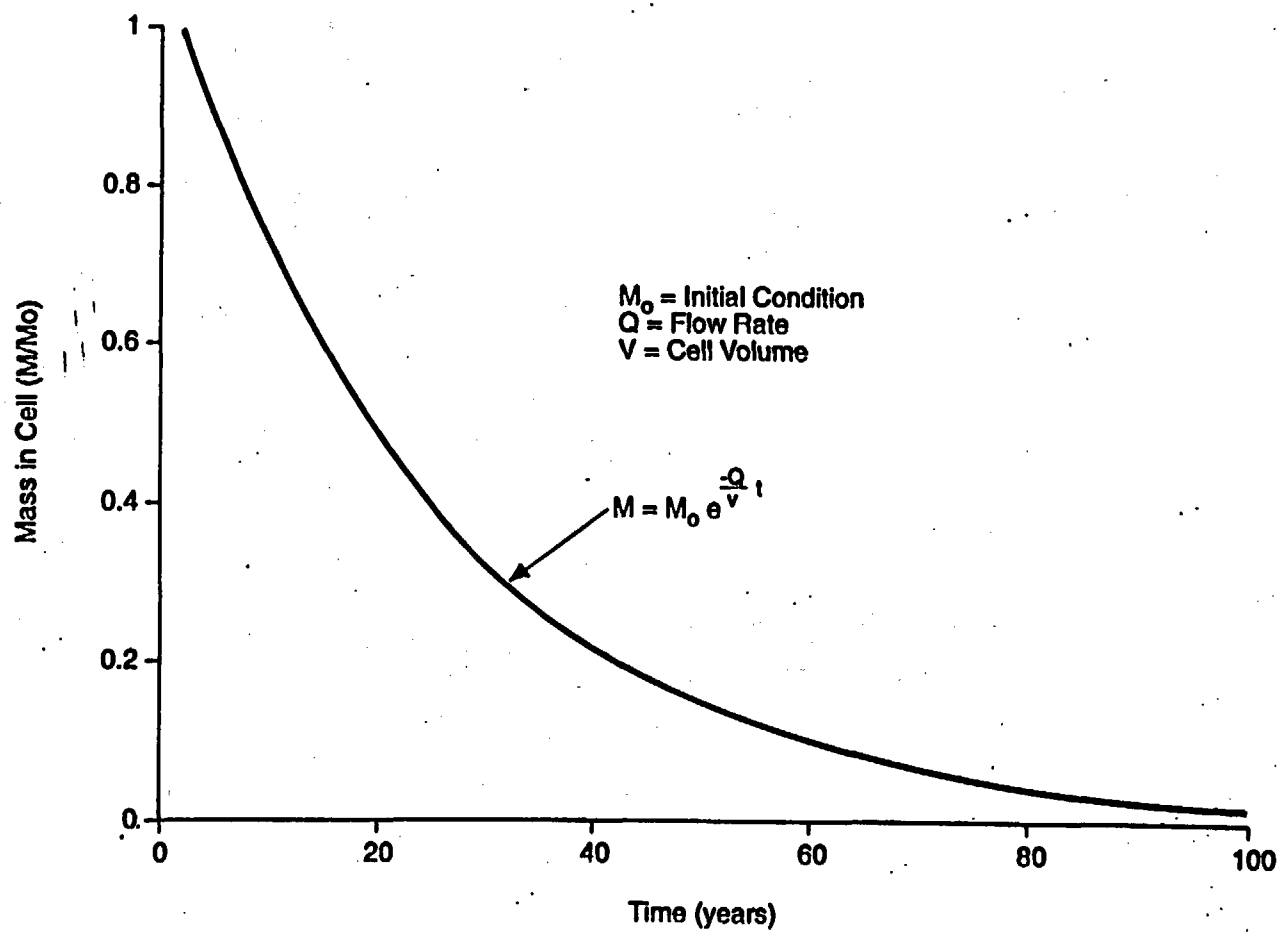


FIGURE 3-5
BEHAVIOR OF SIMPLE MIXING CELL

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# Diffusive Connections

$$f_{cs} = D_{cs}\left(-c_{ims} + \frac{c_{jns}}{K_{nms}}\right) + \sum_{t=1}^{NPT_{im}} PFD_{ct} \cdot D_{ct}\left(-c_{its} \cdot cp_{imt} + c_{jts} \cdot cp_{jnt}\right)$$

$D_{cs}$ = diffusive conductance for species s in connection c

$c_{ims}$ = the dissolved concentration of species s in medium m within cell i

$c_{jns}$ = the dissolved concentration of species s in medium n within cell j

$K_{nms}$ = partition coefficient between fluid medium n (in cell j) and fluid medium m (in cell i) for species s;

$NPT_{im}$ = the number of particulate solid media in fluid m within cell i;

$PFD_{ct}$ = flag if diffusion of solid t suspended in fluid for connection c is allowed

$D_{ct}$ = diffusive conductance for particulate t in connection c

$c_{its}$ = the sorbed or precipitated concentration of species s associated with solid t within cell i

$cp_{imt}$ = the concentration of solid particulate t within fluid m in cell i

$c_{jts}$ = the sorbed or precipitated concentration of species s associated with solid t within cell j

$cp_{jnt}$ = the concentration of solid particulate t within fluid n in cell j .

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# Diffusive Conductance Term

$$D_{cs} = \frac{A_c}{\dfrac{L_{ci}}{d_{ms} \cdot t_{Pci} \cdot n_{Pci}} + \dfrac{L_{cj}}{d_{ns} \cdot t_{Pcj} \cdot n_{Pcj} \cdot K_{nms}}}$$

where:

$L_{ci}$ and $L_{cj}$ are diffusive lengths (m)
$A_c$ is the diffusive area ($m^2$)
$d_{ms}$ and $d_{ns}$ are diffusivities ($m^2/yr$)
$t_{Pci}$ and $t_{Pcj}$ are tortuosities
$n_{Pci}$ and $n_{Pcj}$ are porosities
$K_{nms}$ is a partition coefficient



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# CONC Operator

- Special operator in RIP:

CONC(#path, #medium, #species)

- Returns concentration of specified species in specified medium in specified pathway
- #medium = #TOTAL returns mass instead of concentration
- #species = #element sums over all isotopes

- Potentially very powerful; must be used with care.



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# Pipe Pathways

- **Provide extremely computationally efficient way to simulate fluid conduits**
- **Only single fluid medium**
- **User specifies:**
  - breakthrough curve
  - retardation factors
- **Breakthrough curve specified in one of two ways:**
  - simple 1-D advection/dispersion equation
  - multiple mode Markov process



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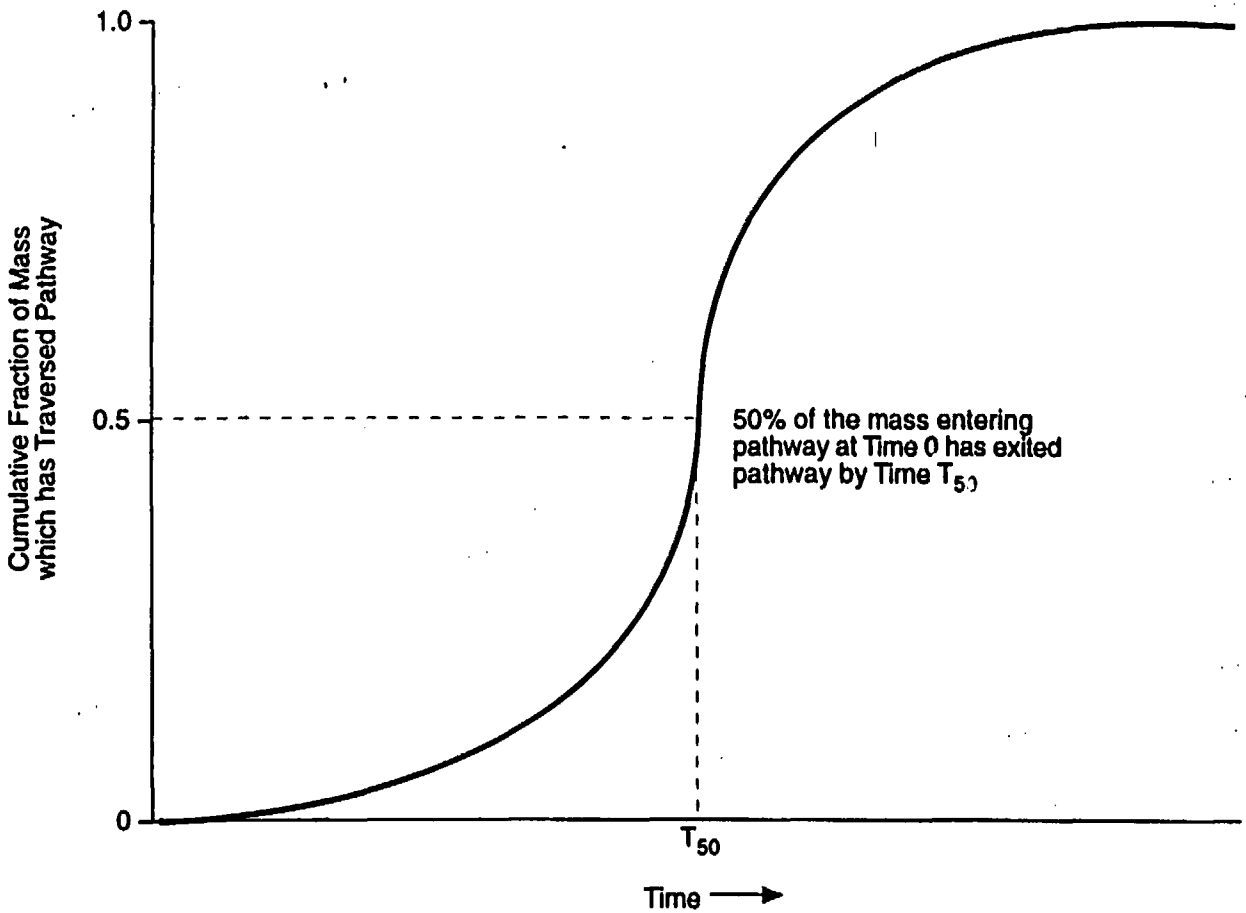


Note: Mass enters pathway as slug at time = 0

FIGURE **3-6**
**PIPE PATHWAY BREAKTHROUGH CURVE**

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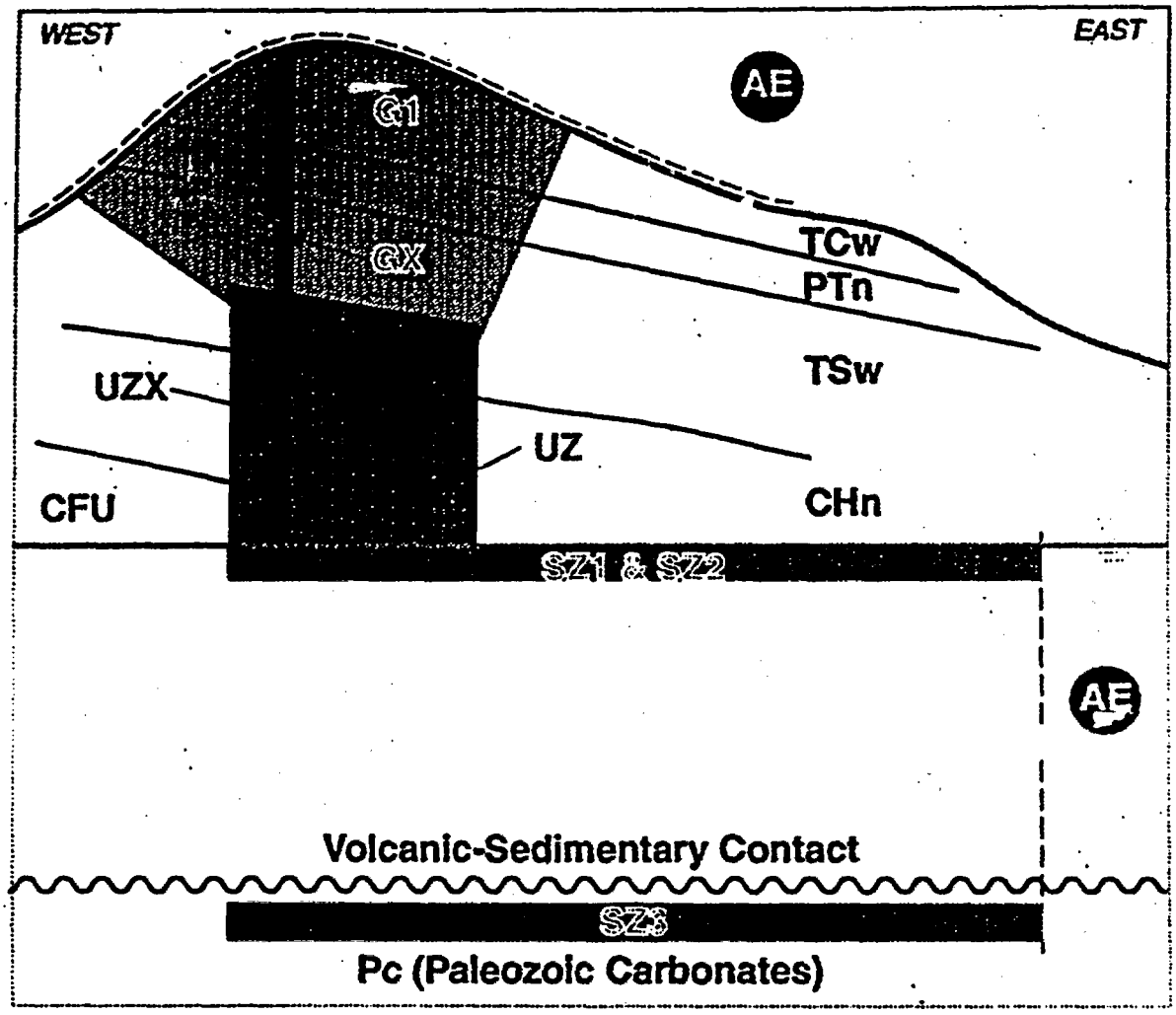
# RIP Pathway Configuration for Yucca Mountain




**Pathway Description**

- Gas Phase
- GX Gas Phase Short Circuit
- UZ Unsaturated Zone (15 Pathways)
- UZX Unsaturated Zone Short Circuit
- SZ1-SZ3 Saturated Zone

AE Accessible Environment

Water Table

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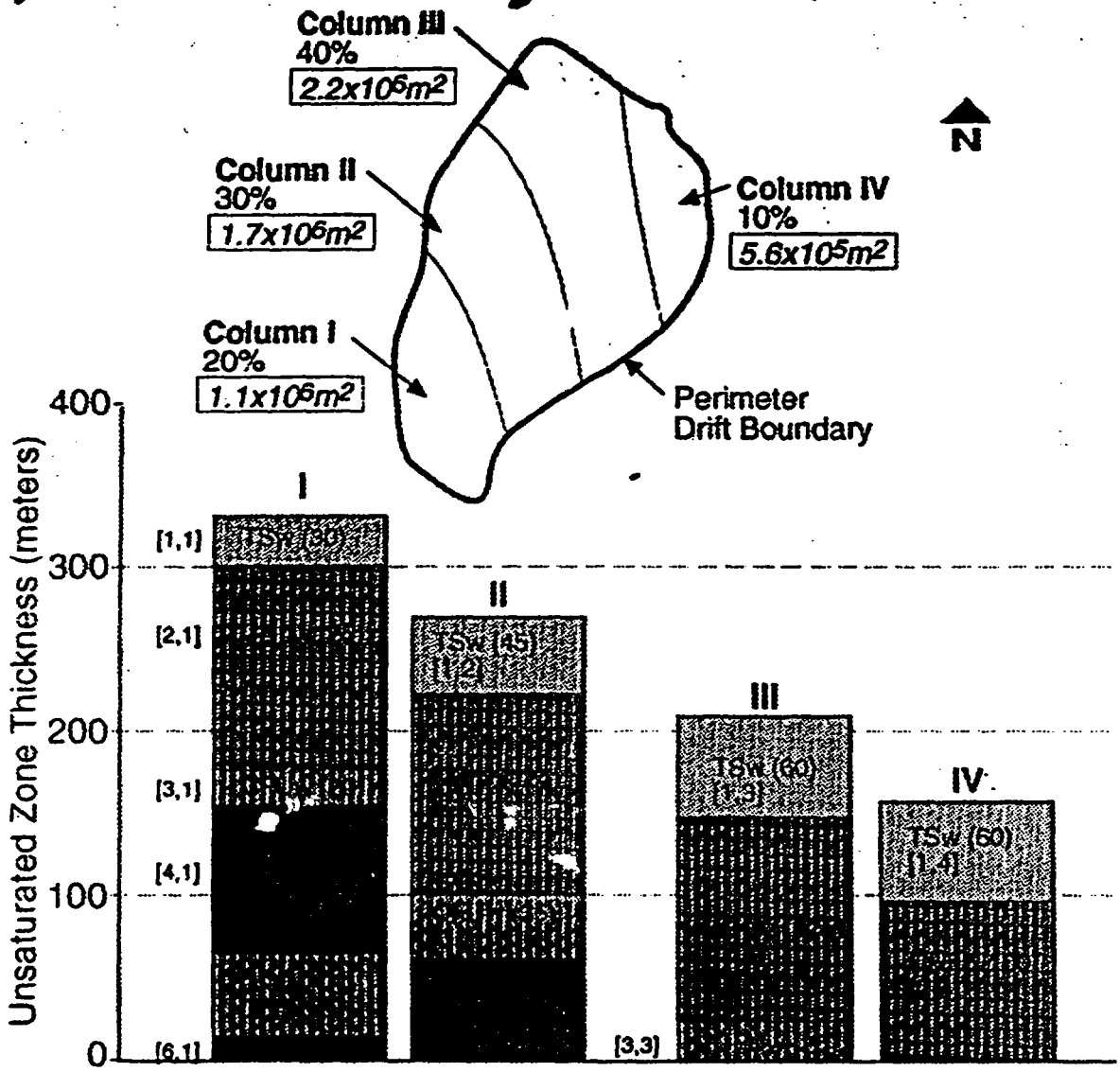
# Unsaturated Zone Pathway Dimensions




CFUn (90) - Hydrologic Unit and Thickness in meters

[2,1] - Unsaturated Zone Pathway index

20% - Area proportion for Pathway Column

$\boxed{1.1x10^6m^2}$ - Pathway Column area

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923-1196-44670/vg/1-26-93

# One-Dimensional Advective/Dispersive Breakthrough Curve

- **User specifies:**
  - transport velocity
  - dispersivity
  - pathway length
- **Transport velocity can be:**
  - specified directly; or
  - computed based on specified values for flow rates, porosity and area:

$$v = Q/(nA)$$



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# Markov Process Breakthrough Curve

- **Define multiple flow modes and solute transition rate between flow modes**
- **Breakthrough curve determined by following relationships:**
  - probability of particle being in a flow mode is proportional to flow in that mode
  - length traveled in a mode follows a Poisson distribution
  - Pr(from i to k) = $f_k$ / (1-$f_i$)



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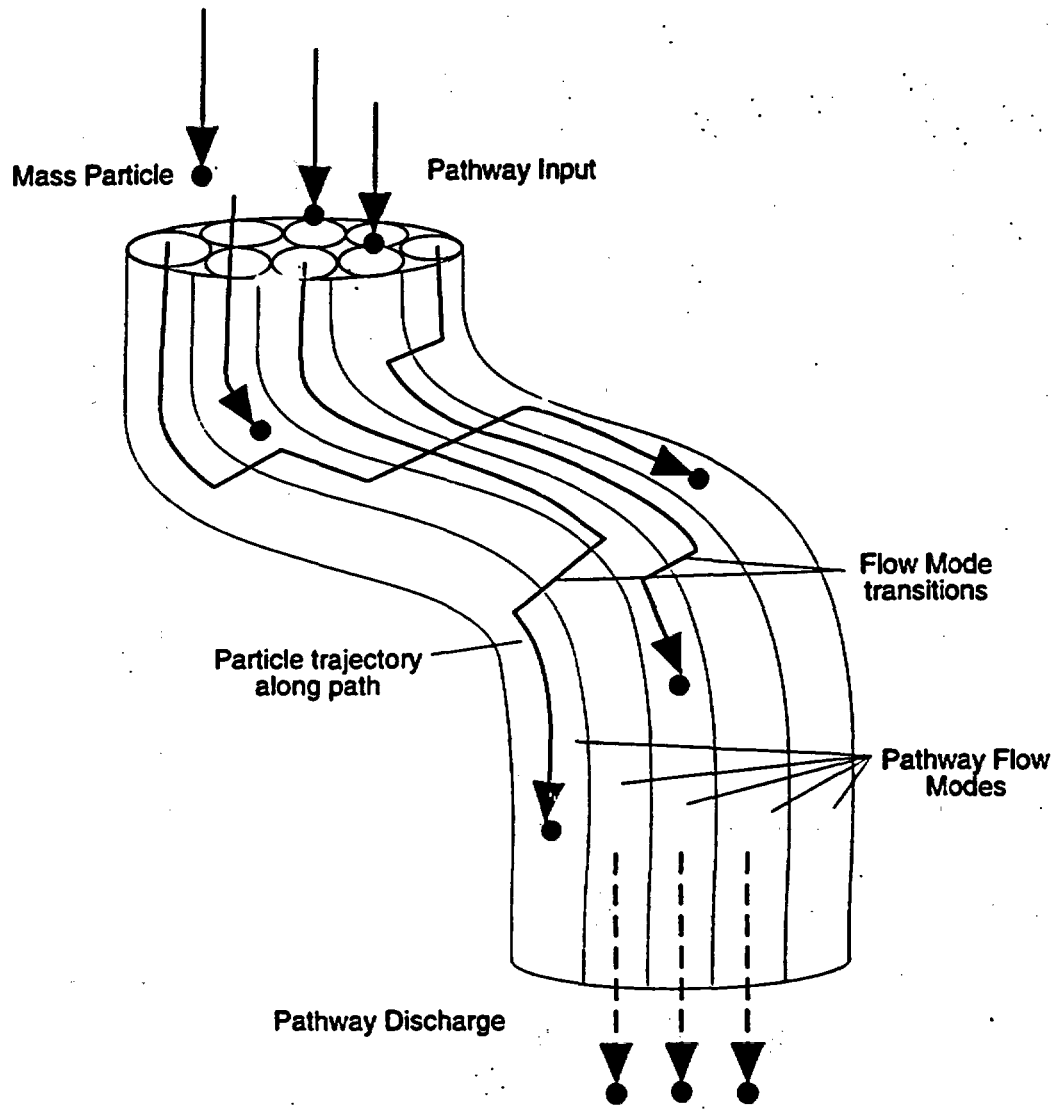


FIGURE 9-5
SCHEMATIC OF MARKOV PROCESS ALGORITHM

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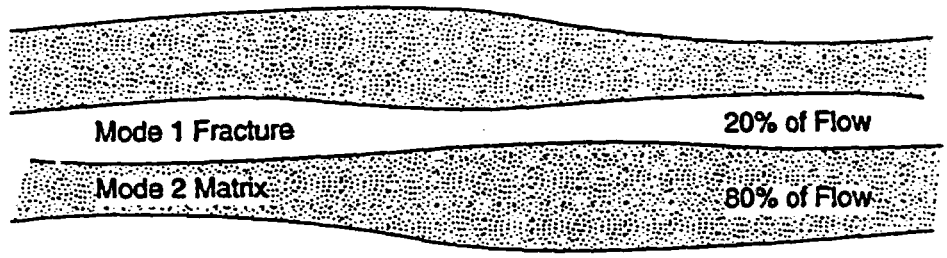


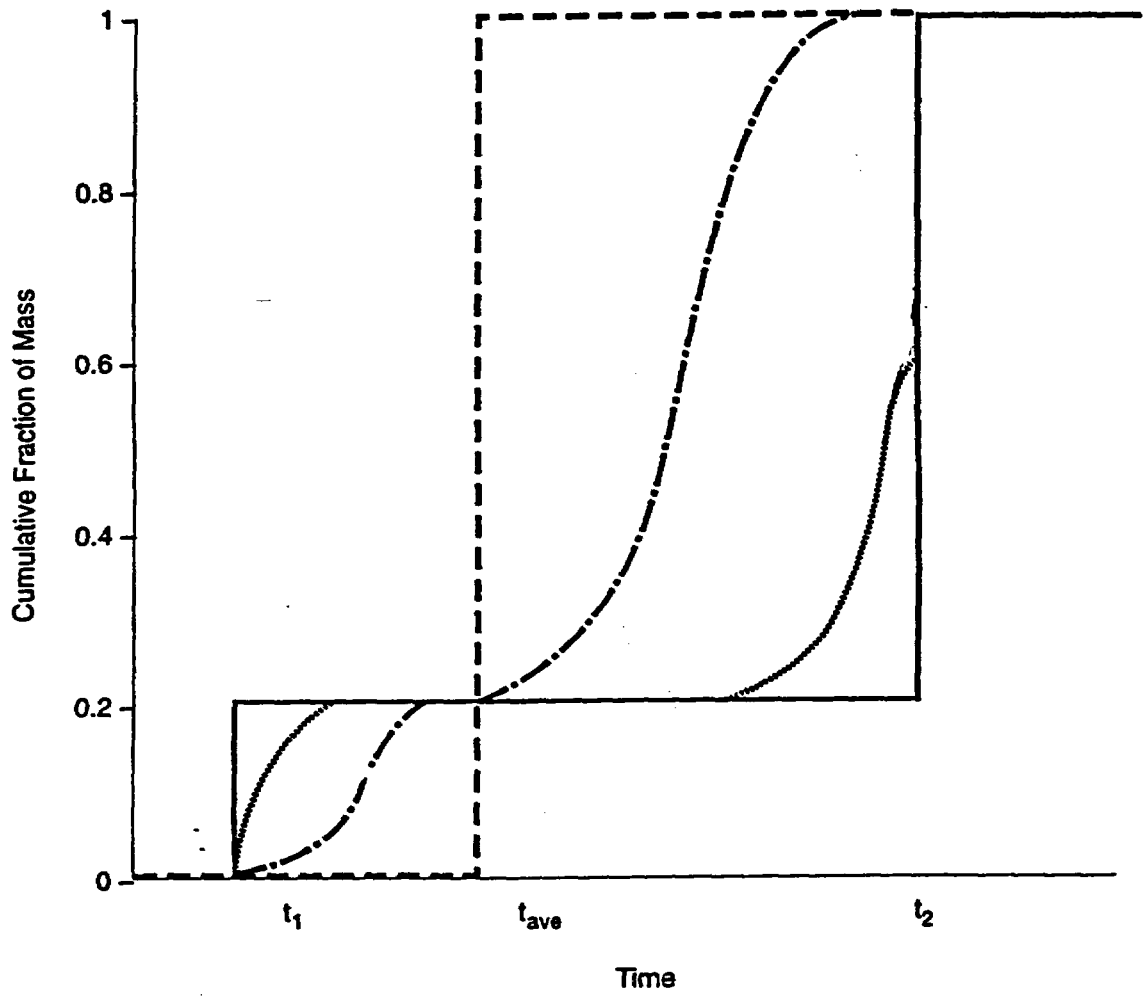


$$t_{ave} = \frac{L}{\sum_i v_i f_i}$$

LEGEND

- Zero Transition Rate
- Infinite Transition Rate
- Low Transition Rate
- Moderate Transition Rate

FIGURE **9-6**

**MULTIPLE MODE MARKOV PROCESS BREAKTHROUGH CURVES**

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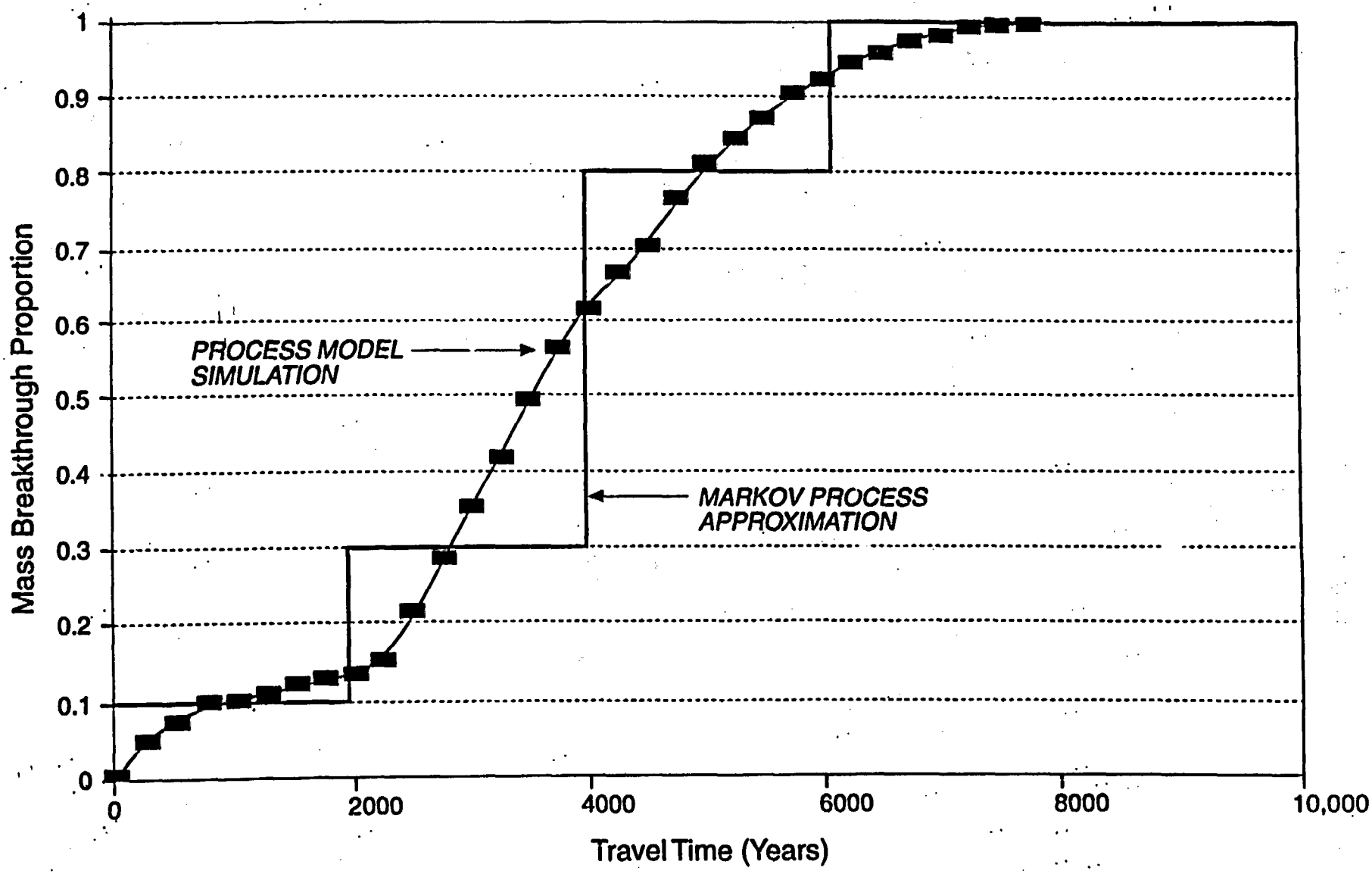


*(adapted from Ross et al. 1991)*

FIGURE **9-7**

**APPROXIMATING COMPLEX BREAKTHROUGH CURVES USING MULTIPLE-MODE MARKOV PROCESS**

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# Mass Transport Algorithm

- In order to computationally track the breakthrough of radionuclides, the program makes some approximations to speed execution
- this results in numerical dispersion



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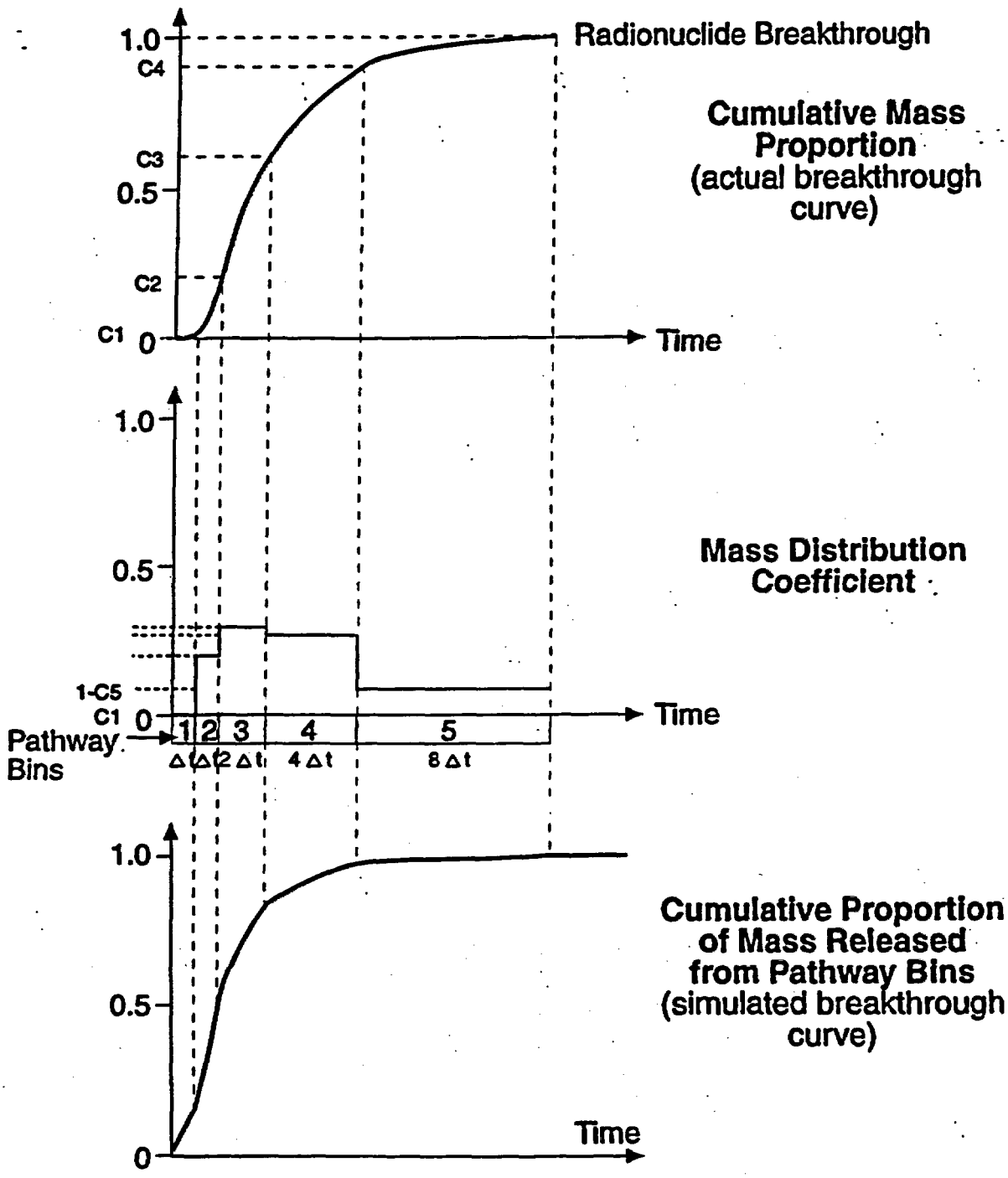


FIGURE **9-8**
**MAPPING OF BREAKTHROUGH CURVE ONTO PIPE PATHWAY BINS**

# Pipe Binning Algorithm

| | $\Delta t$ = 10 years | $\Delta t$ = 50 years | $\Delta t$ = 100 years |
|---|---|---|---|
| bin | Pathway Entry Residence Time (years) | Pathway Entry Residence Time (years) | Pathway Entry Residence Time (years) |
| 1 | 0 - 10 | 0 - 50 | 0 - 100 |
| 2 | 10 - 20 | 50 - 100 | 100 - 200 |
| 3 | 20 - 40 | 100 - 200 | 200 - 400 |
| 4 | 40 - 80 | 200 - 400 | 400 - 800 |
| 5 | 80 - 160 | 400 - 800 | 800 - 1600 |
| 6 | 160 - 320 | 800 - 1600 | 1600 - 3200 |
| 7 | 320 - 640 | 1600 - 3200 | 3200 - 6,400 |
| 8 | 640 - 1,280 | 3200 - 6,400 | 6400 - 12,800 |
| 9 | 1,280 - 2,560 | 6400 - 12,800 | 12,800 - 25,600 |
| 10 | 2,560 - 5,120 | 12,800 - 25,600 | |
| 11 | 5,120 - 10,240 | | |
| 12 | 10,240 - 20,480 | | |



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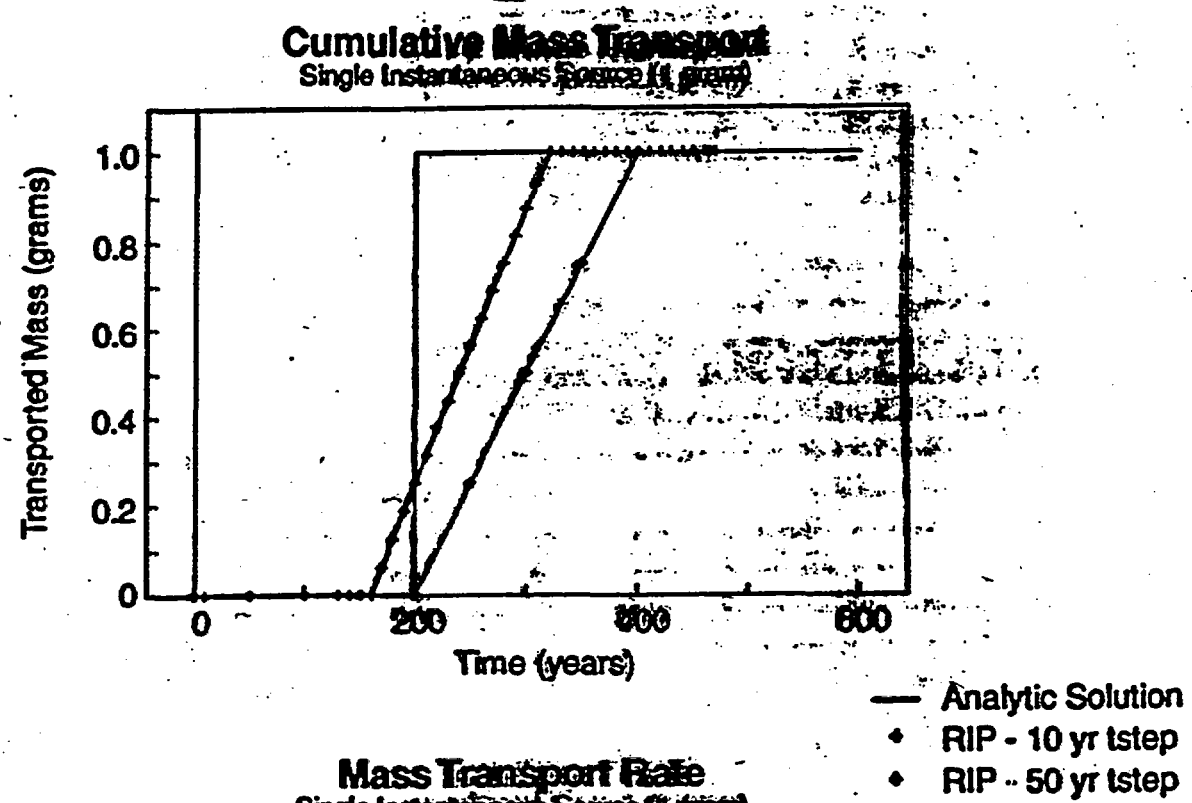
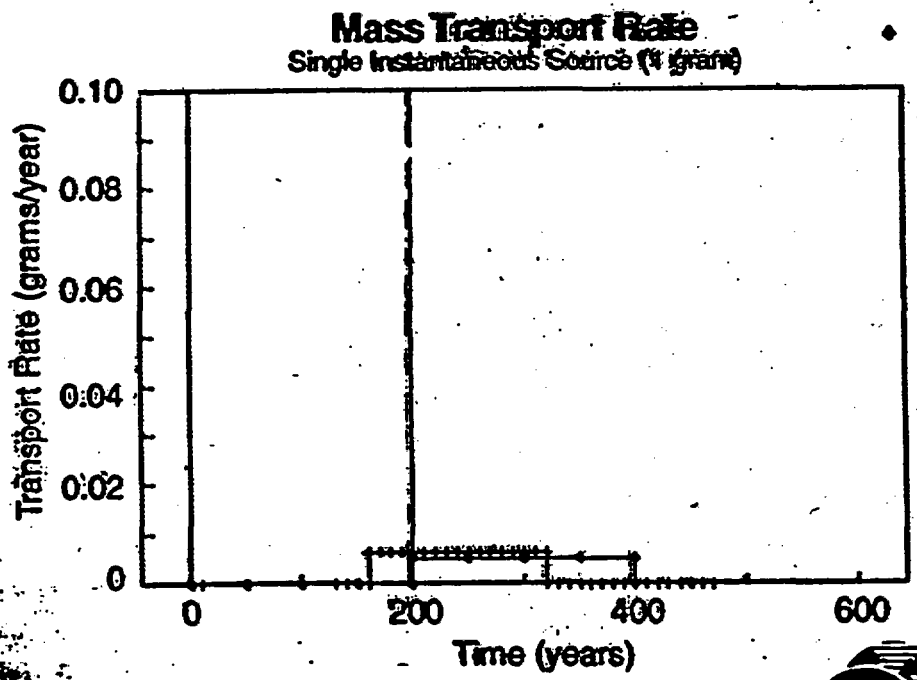
# Slug Input With No Dispersion

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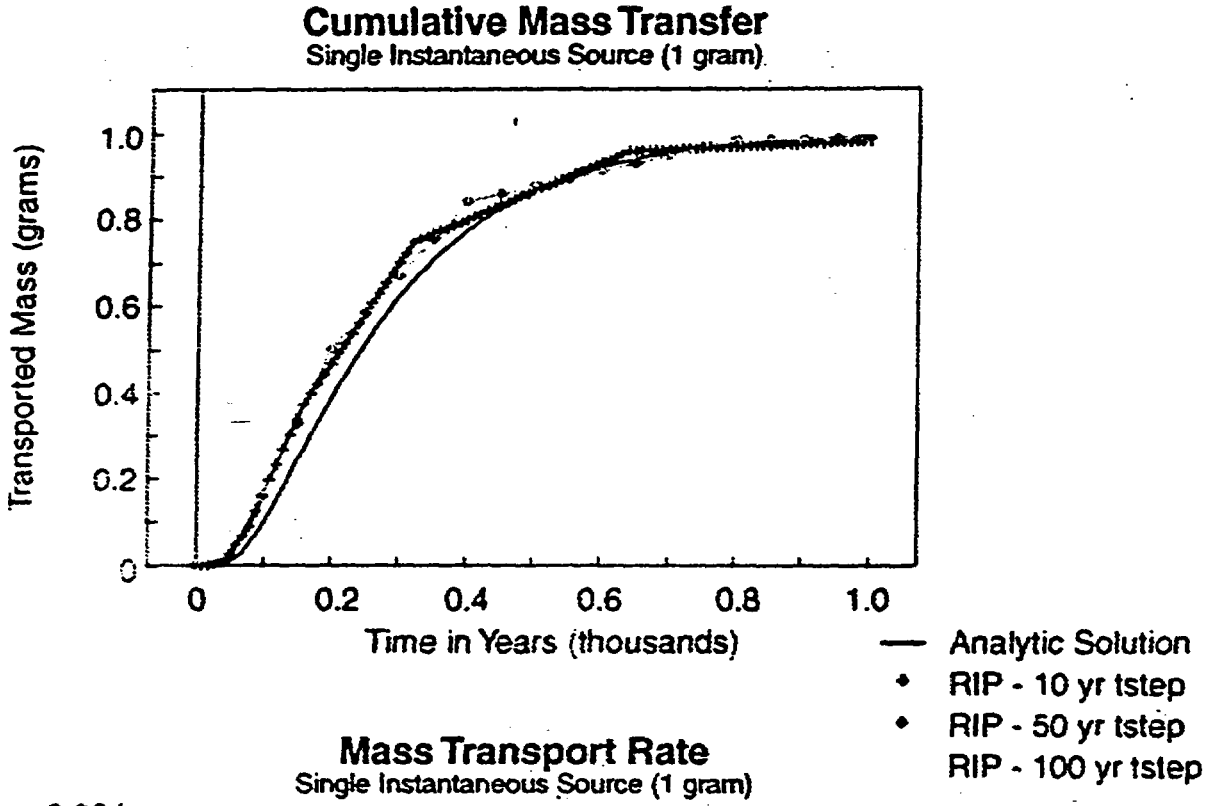
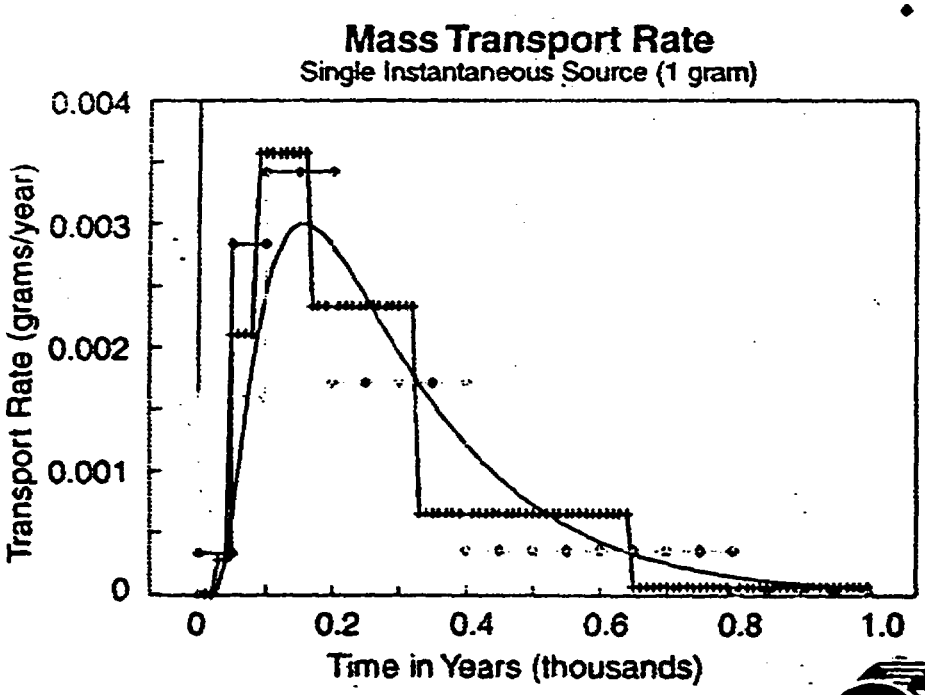
# Slug Input With Dispersion

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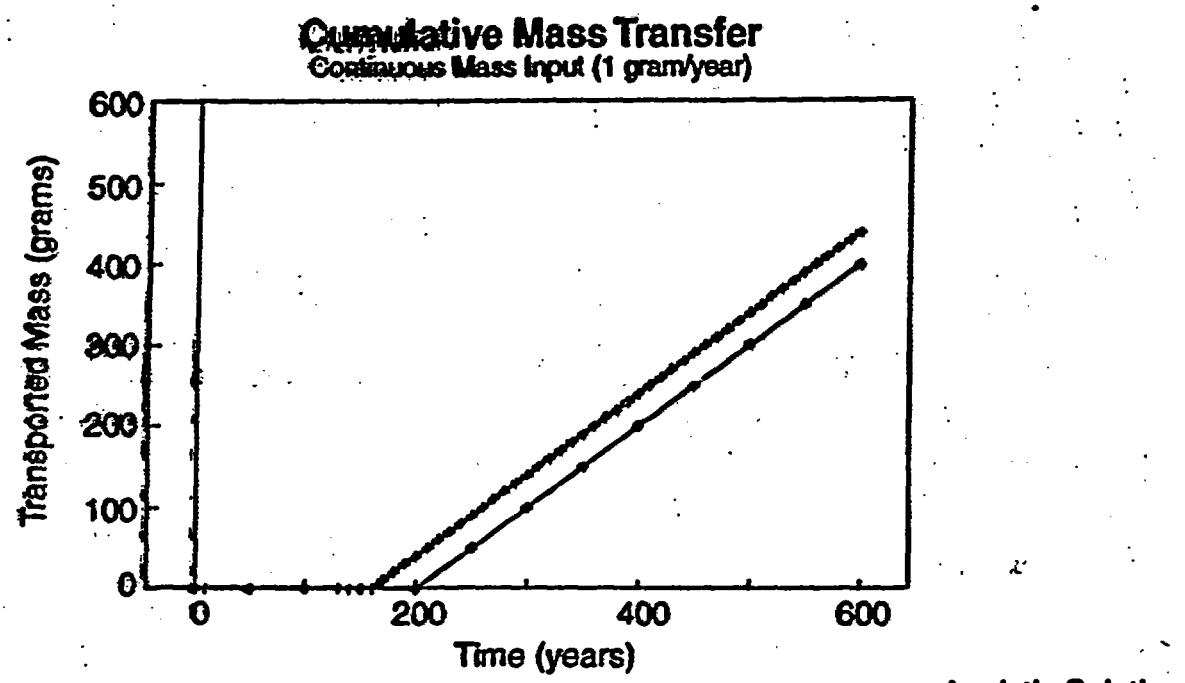
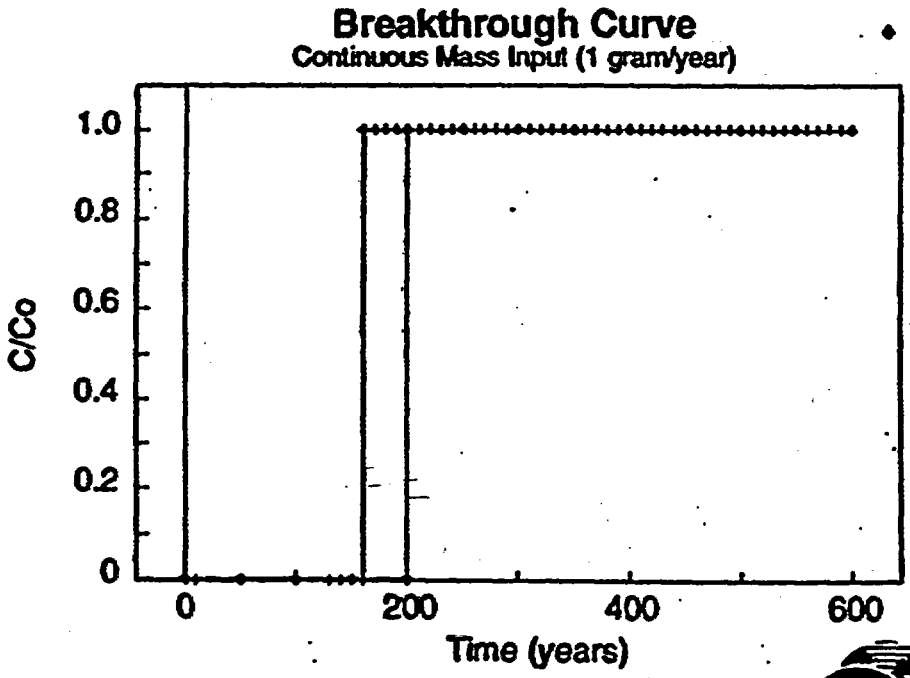
# Constant Input With No Dispersion

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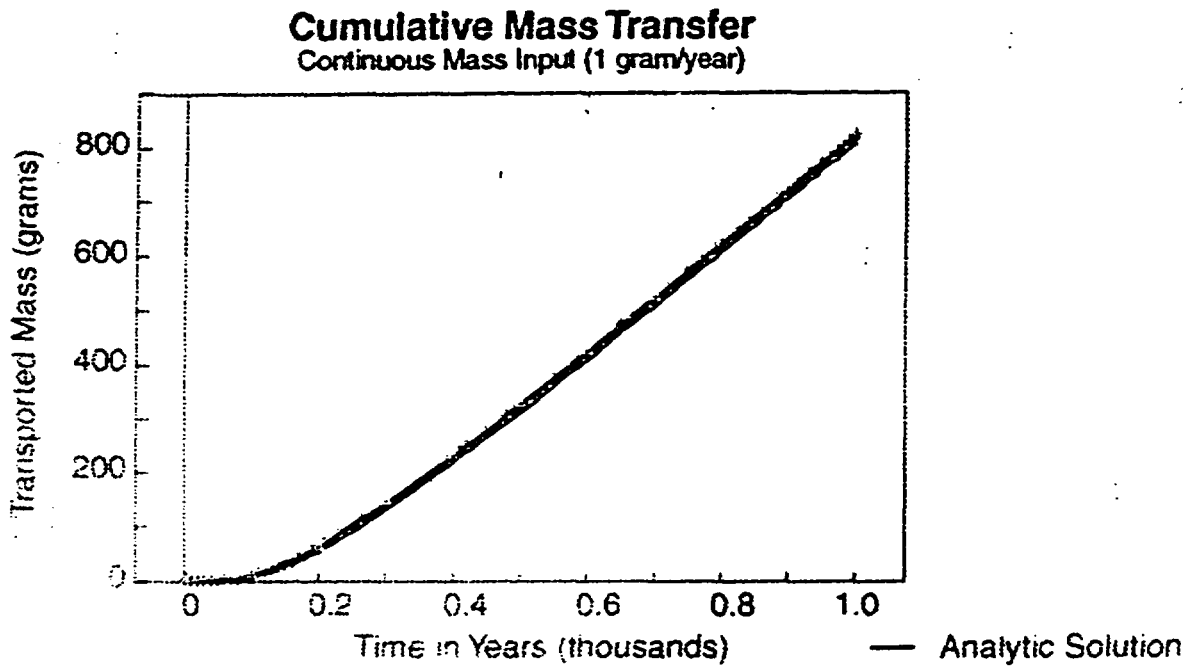
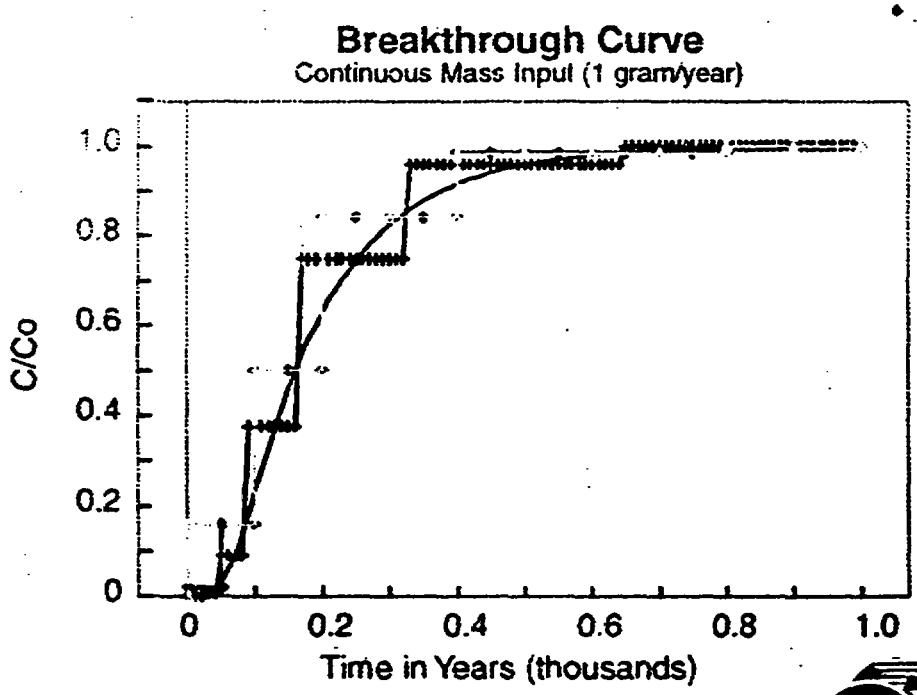
# Constant Input With Dispersion

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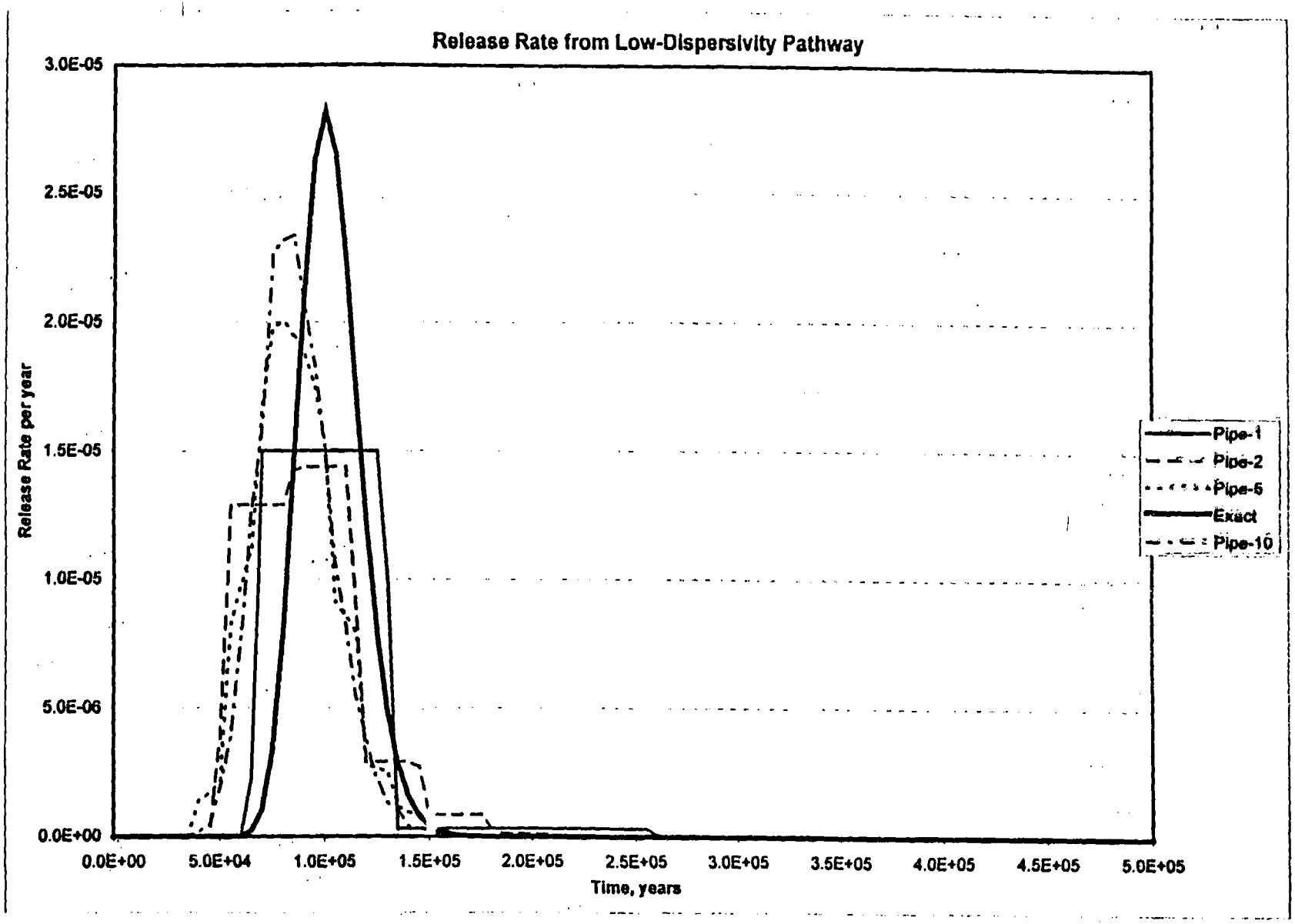
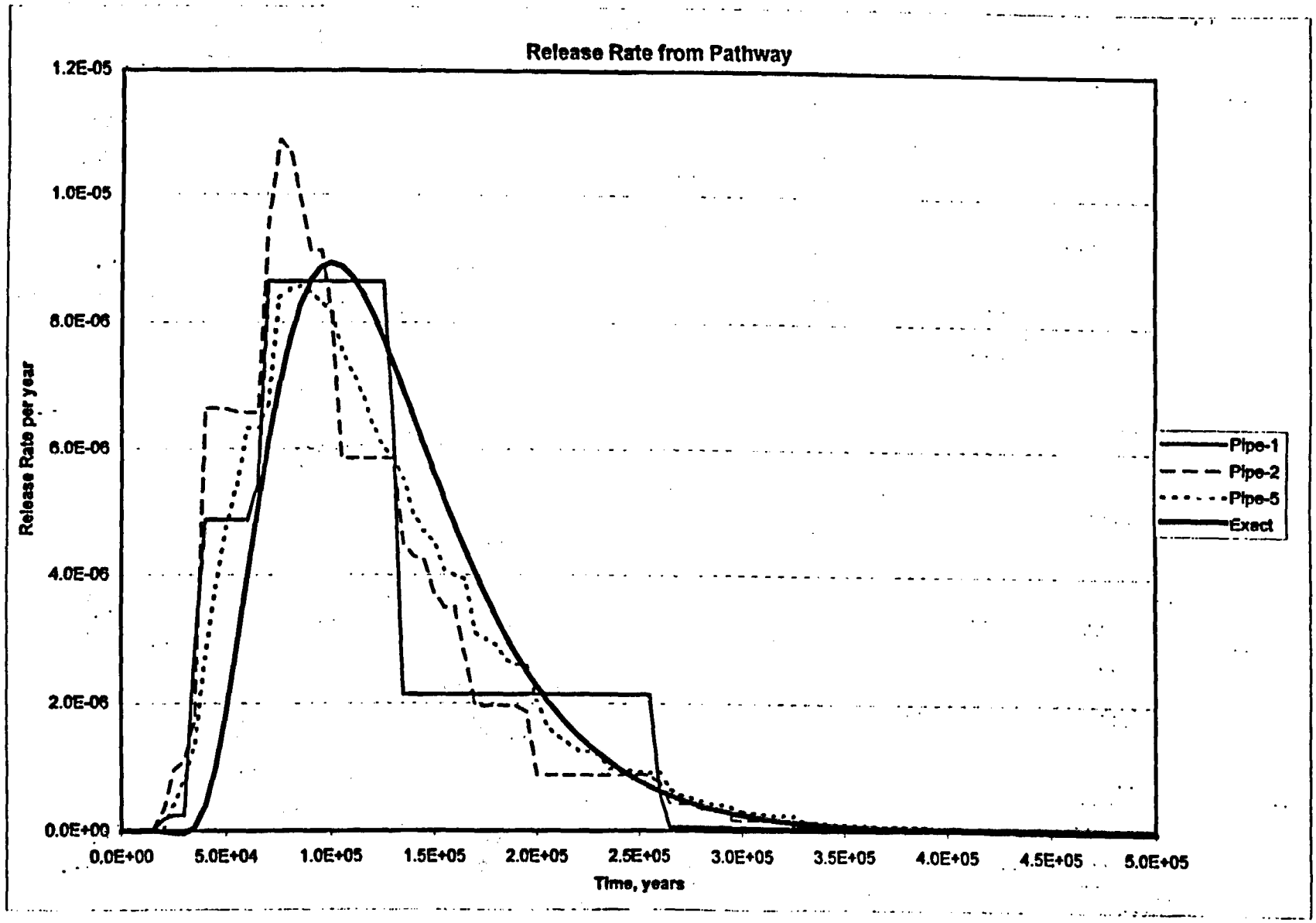
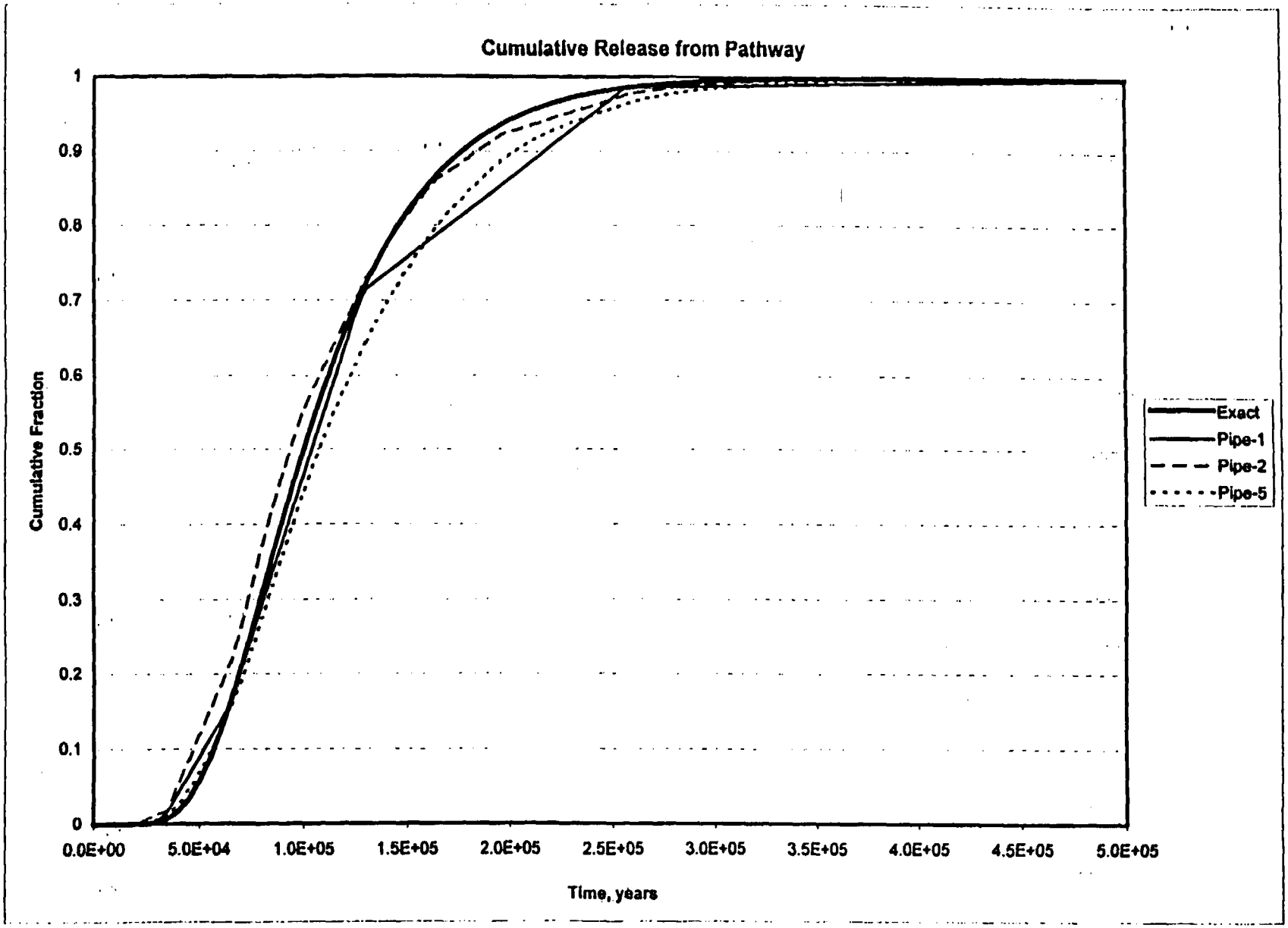
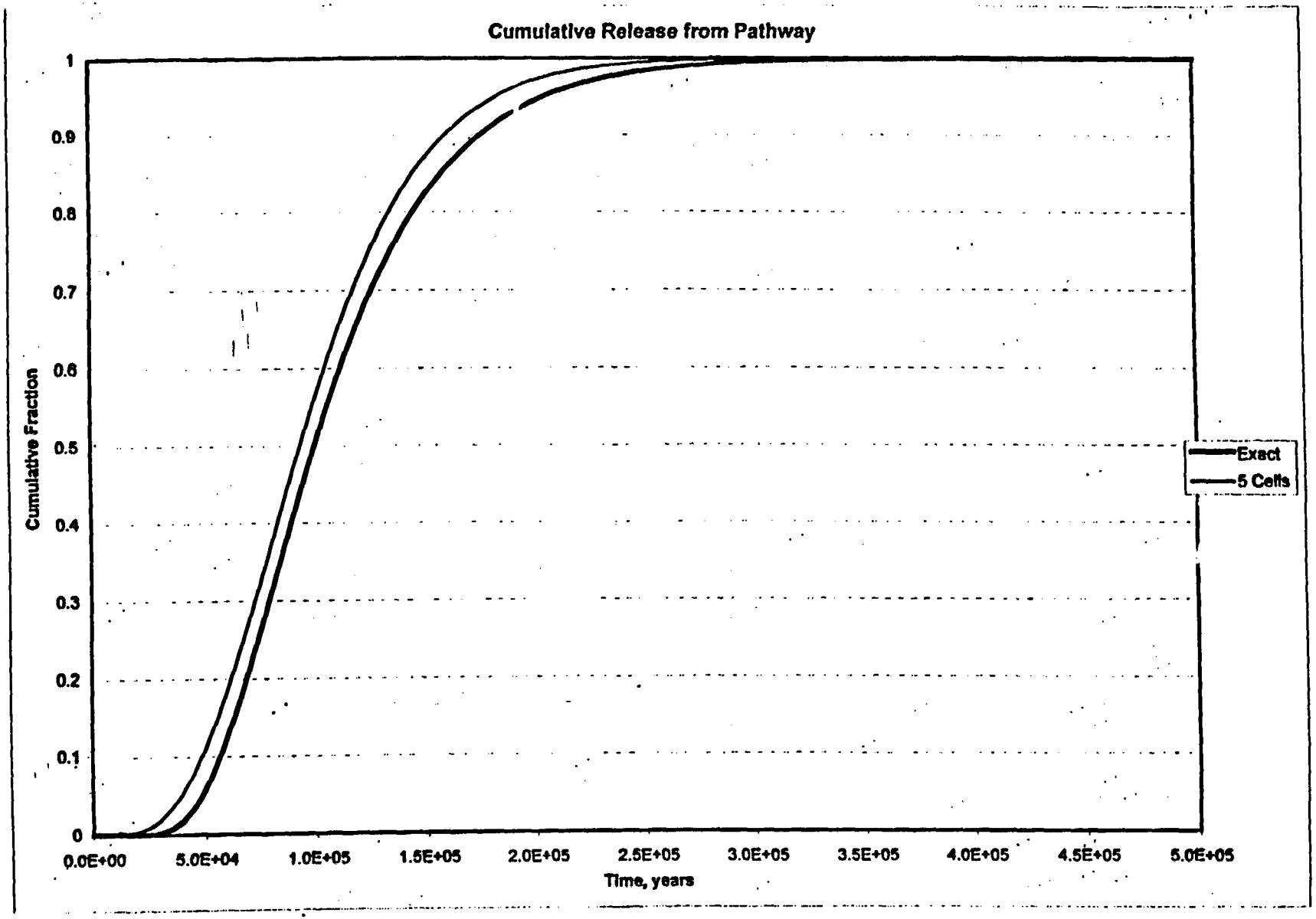
# Sub-Dividing a Pipe

- **Pipe pathways can be automatically sub-divided (spatially discretized).**
- **This has two benefits:**
  - "smoothes" out curves (primarily cosmetic)
  - reduces error incurred due to daughter product ingrowth:
    - **daughters must move with parent until discharged from the pathway in which they were created**


Release Rate from Low-Dispersivity Pathway
Release Rate per year
3.0E-05
2.5E-05
2.0E-05
1.5E-05
1.0E-05
5.0E-06
0.0E+00
0.0E+00
5.0E+04
1.0E+05
1.5E+05
2.0E+05
2.5E+05
3.0E+05
3.5E+05
4.0E+05
4.5E+05
5.0E+05
Time, years
Pipe-1
Pipe-2
Pipe-5
Exact
Pipe-10


Release Rate from Pathway
1.2E-05
1.0E-05
8.0E-06
6.0E-06
4.0E-06
2.0E-06
0.0E+00
Release Rate per year
0.0E+00
5.0E+04
1.0E+05
1.5E+05
2.0E+05
2.5E+05
3.0E+05
3.5E+05
4.0E+05
4.5E+05
5.0E+05
Time, years
Pipe-1
Pipe-2
Pipe-5
Exact


Cumulative Release from Pathway
Cumulative Fraction
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.0E+00
5.0E+04
1.0E+05
1.5E+05
2.0E+05
2.5E+05
3.0E+05
3.5E+05
4.0E+05
4.5E+05
5.0E+05
Time, years
Exact
Pipe-1
Pipe-2
Pipe-5


Cumulative Release from Pathway
Cumulative Fraction
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.0E+00
5.0E+04
1.0E+05
1.5E+05
2.0E+05
2.5E+05
3.0E+05
3.5E+05
4.0E+05
4.5E+05
5.0E+05
Time, years
Exact
5 Cells

# Implementing Temporal Changes to a Breakthrough Curve

- Parameters describing breakthrough curve can be time variable
- Mass already in pathway is not affected
- Shortening a pathway has special consequences
- User can define tolerance values to control how breakthrough changes are represented



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# Computing Concentration for a Geosphere Pathway

- $$C_{rj} = \frac{M_{rj}}{\sum_{i=1}^{fmodes} (L_j A_j n_i R_{jri})}$$

- where:

$M_{rj}$ = mass of radionuclide r in pathway j (g)

$L_j$ = length of pathway j (m)

$A_j$ = cross-sectional area of pathway j ($m^2$)

$n_{ji}$ = effective porosity of flow mode i in pathway j

$R_{jri}$ = retardation factor for radionuclide r in pathway j, flow mode i



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# External Pathways

- **Provides mechanism for linking external solute transport models directly into RIP**
- **Required steps:**
  - code and compile external pathway function
  - specify name of function being used to simulate external pathway
  - specify linkages into pathway network
  - specify additional arguments to send to function
  - link function to RIP at run-time
  - RIP calls function every timestep



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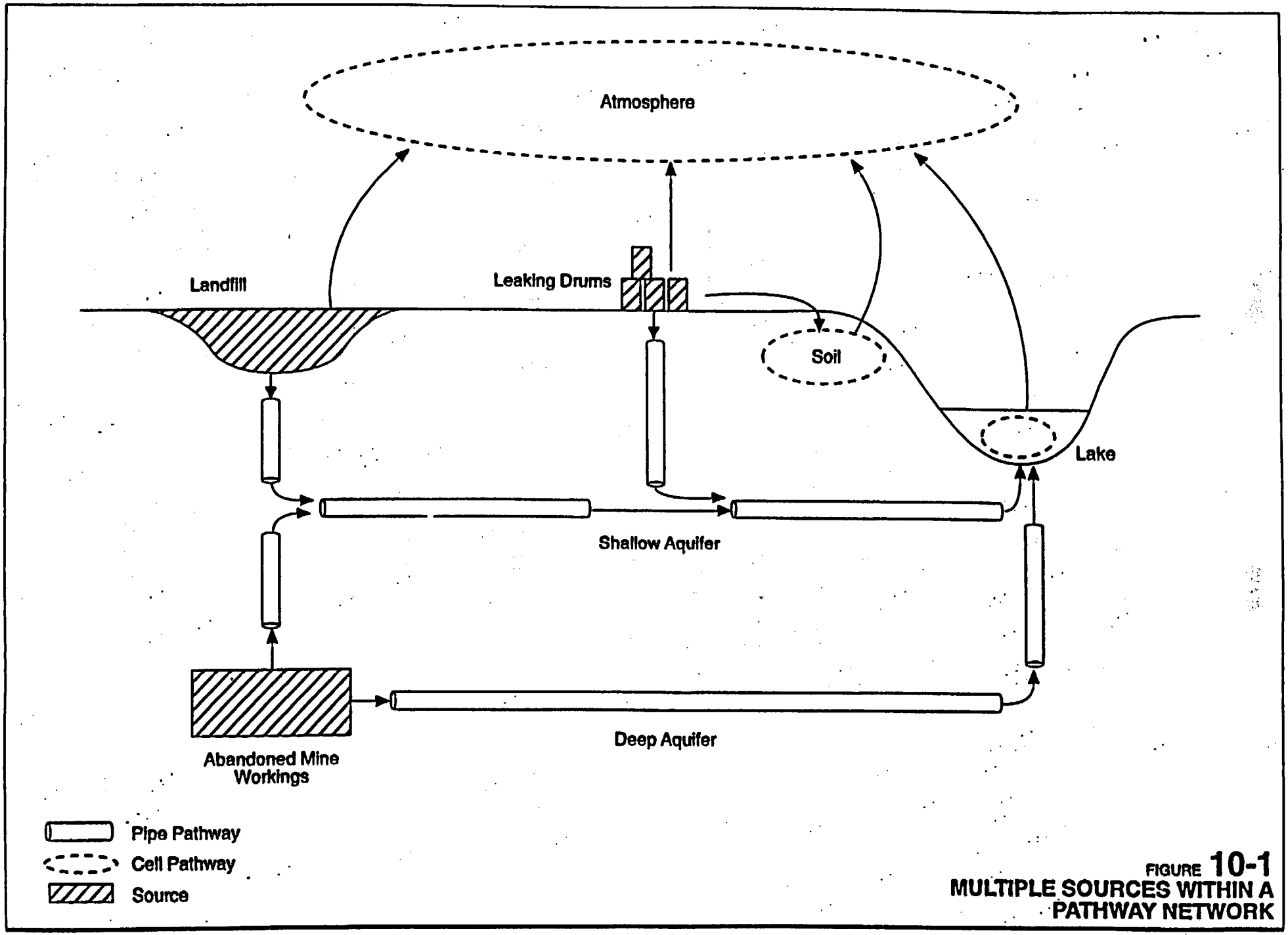


FIGURE 10-1
MULTIPLE SOURCES WITHIN A PATHWAY NETWORK

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# Properties and Characteristics of a Source

- Inventory
- Containment layers
- Waste matrix
- Mass transfer
- Connections to pathway network

Mechanisms controlling release:

- mass exposure
- transport of exposed mass



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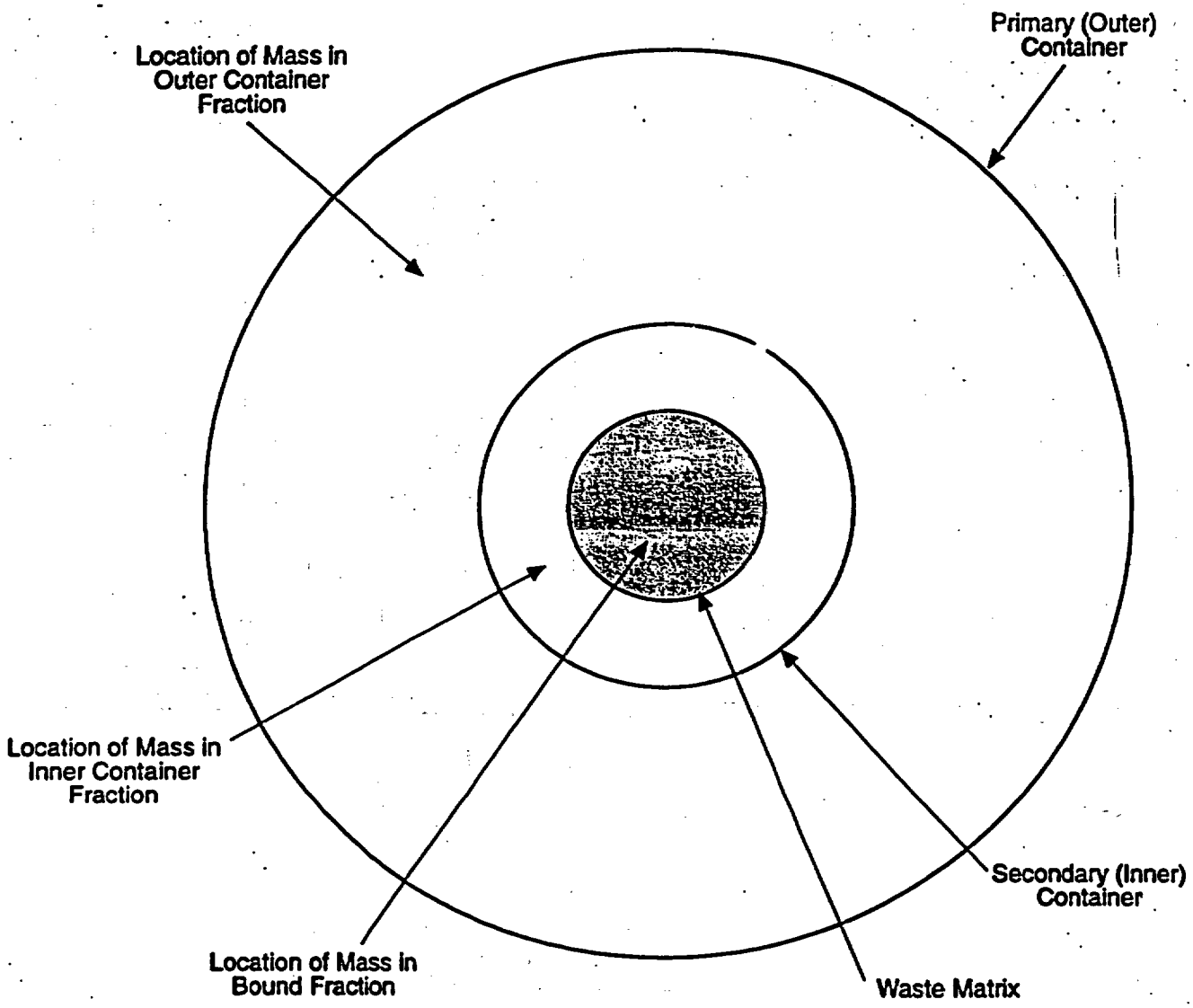


FIGURE 10-3
CONTAINER COMPONENTS

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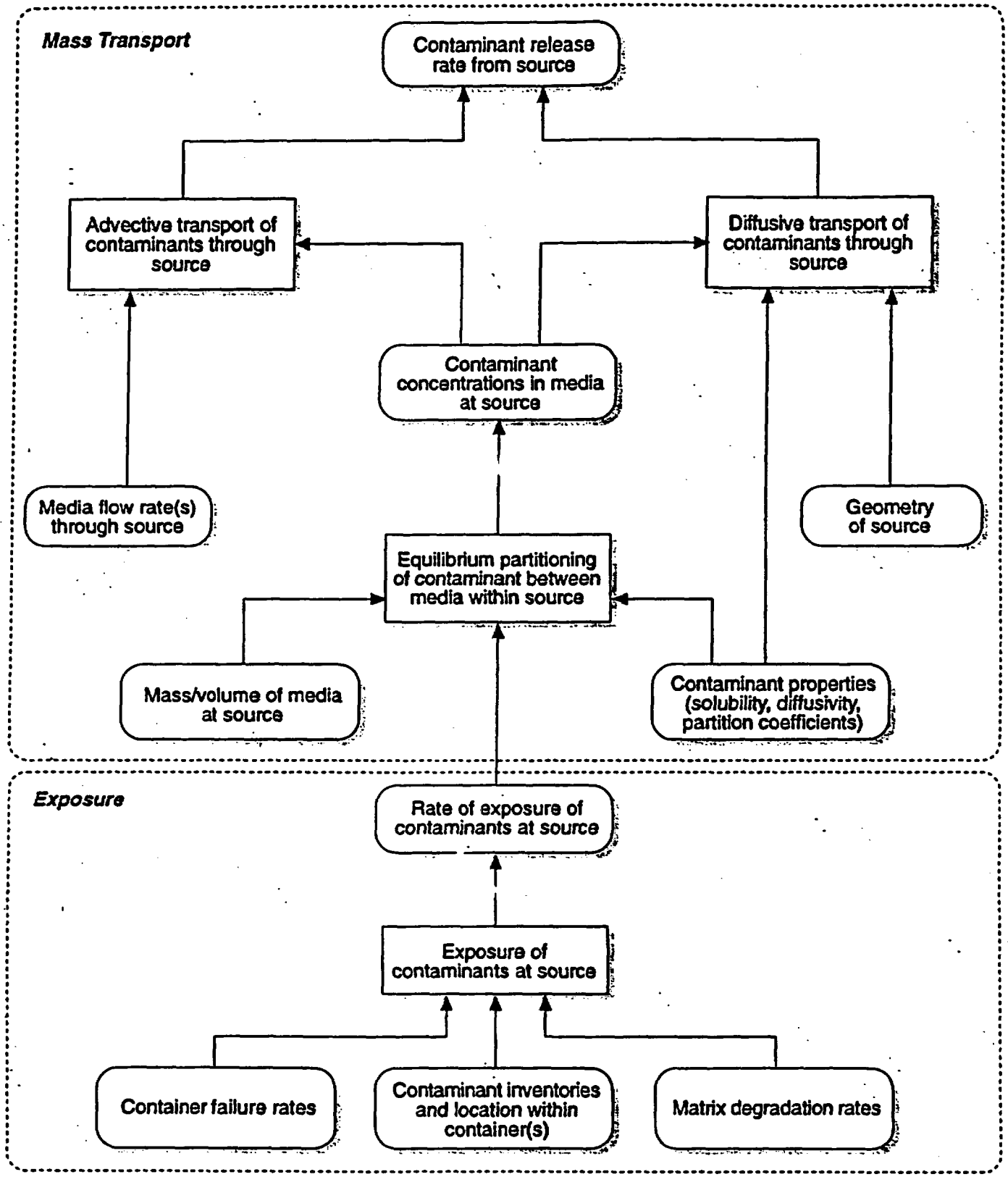


FIGURE **10-2**
**SOURCE TERM MODEL SCHEMATIC**

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# Mass Exposure

- Exposure is brought about by failure of containers and degradation of any waste matrix in which mass is bound
- Exposed implies mass is available for mass transport
- Exposure rates are computed as functions of container failure rates and degradation rates

# Container Failure

- **Can specify variety of failure distributions**
  - Weibull
  - exponential
  - uniform
  - log-uniform
  - degenerate
  - user-defined
- **Primary failure can be linked to a specified condition**
- **Secondary failure can be linked to primary failure**
- **RIP combines failure modes assuming no synergism**

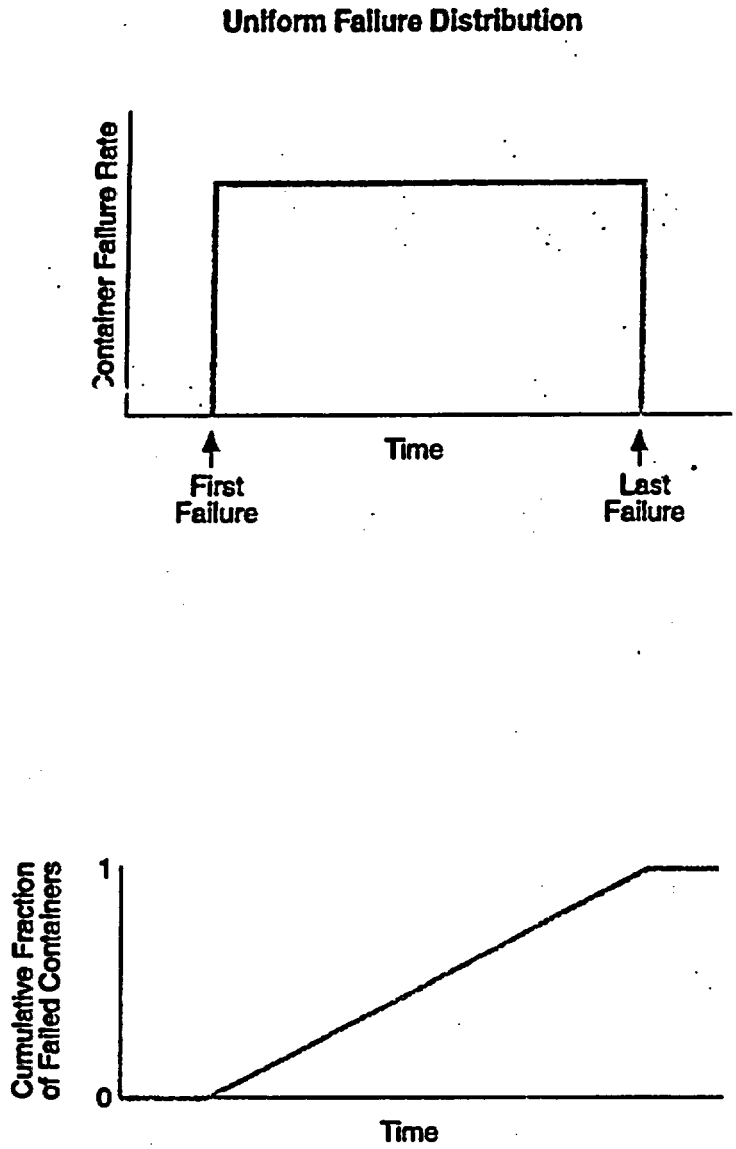


FIGURE 3-2
SOURCE TERM CONTAINER FAILURE DISTRIBUTION

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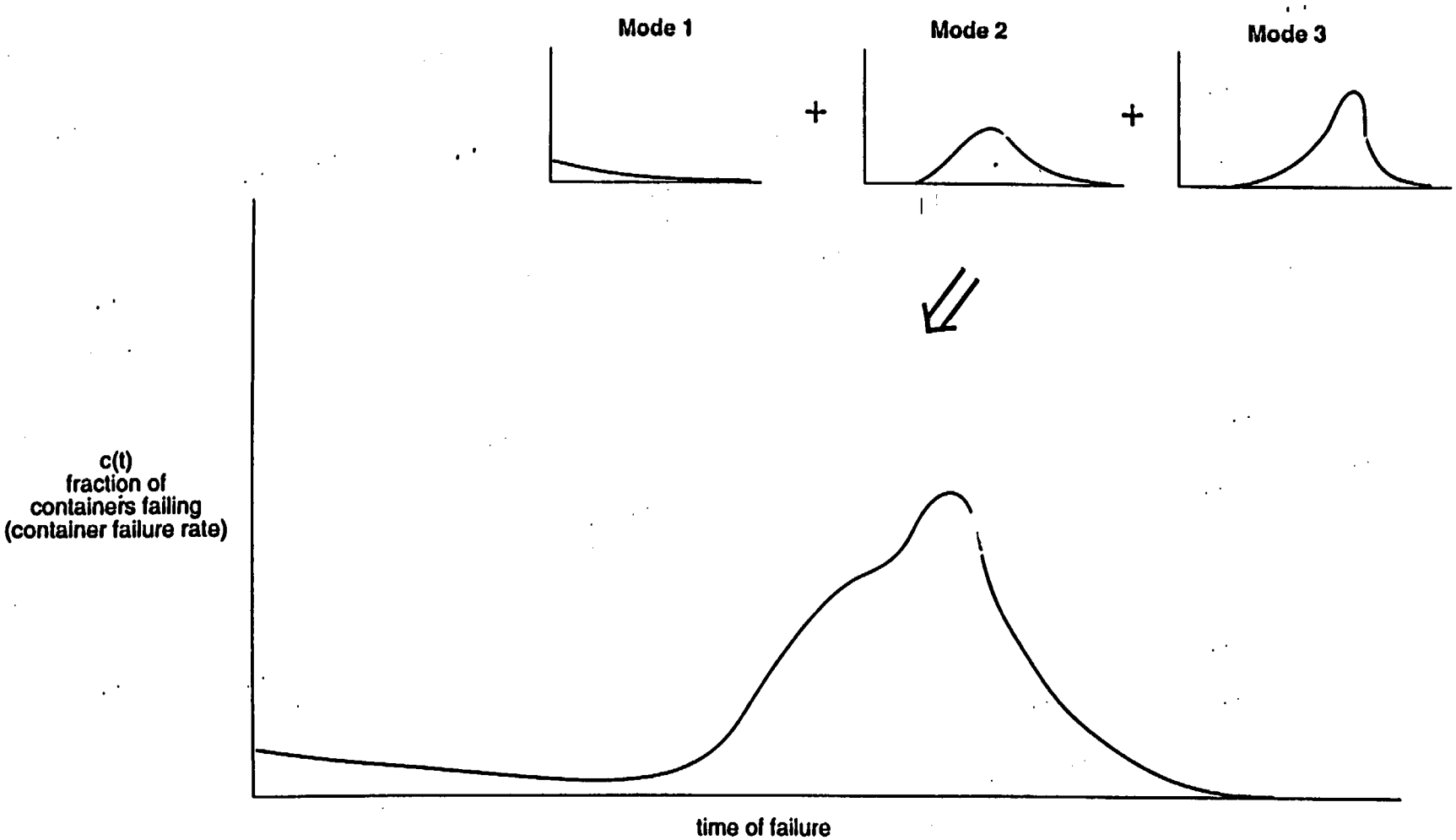


FIGURE 10-4
CONTAINER FAILURE DISTRIBUTIONS

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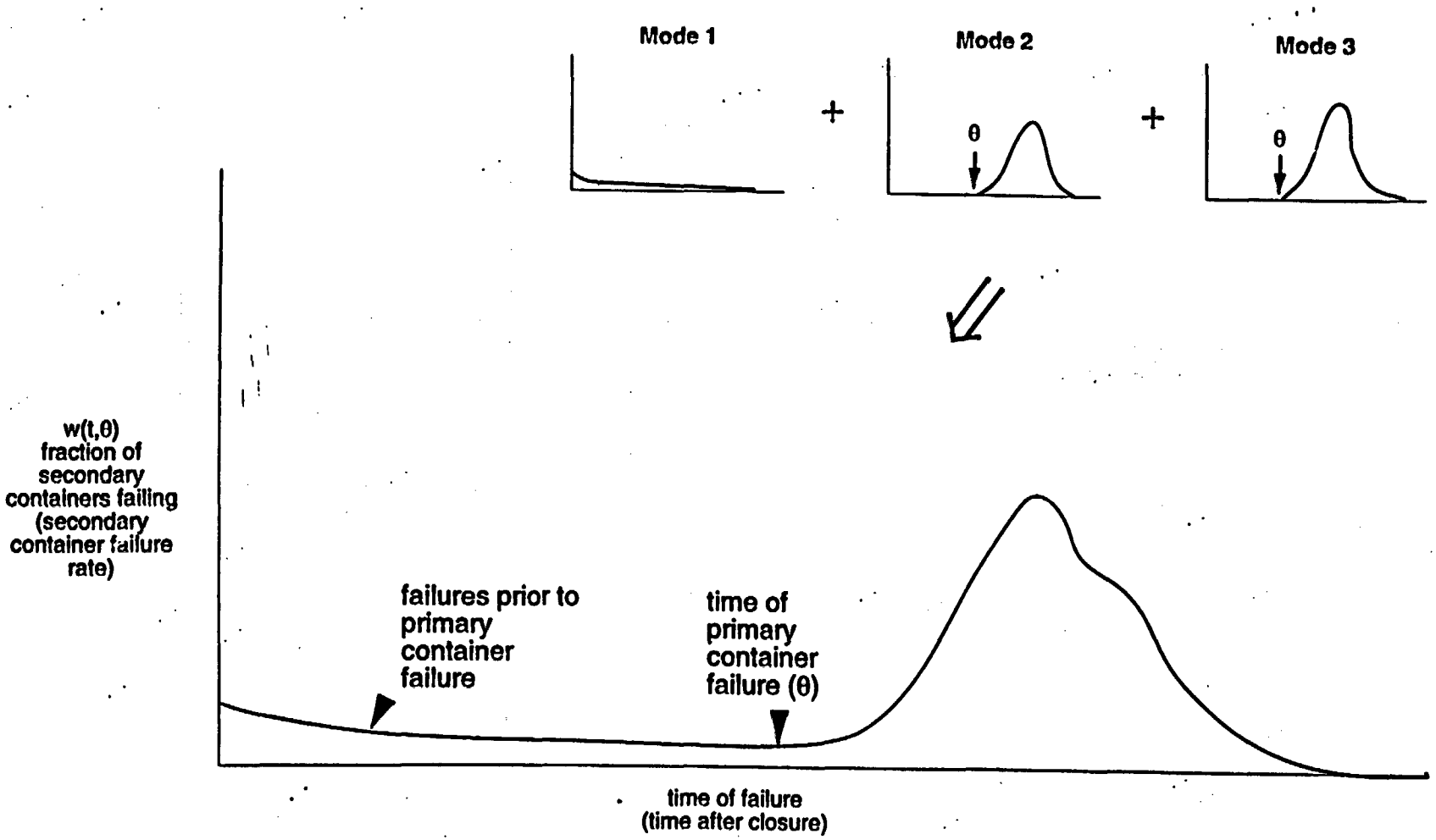


FIGURE 10-6
SECONDARY CONTAINER FAILURE DISTRIBUTION

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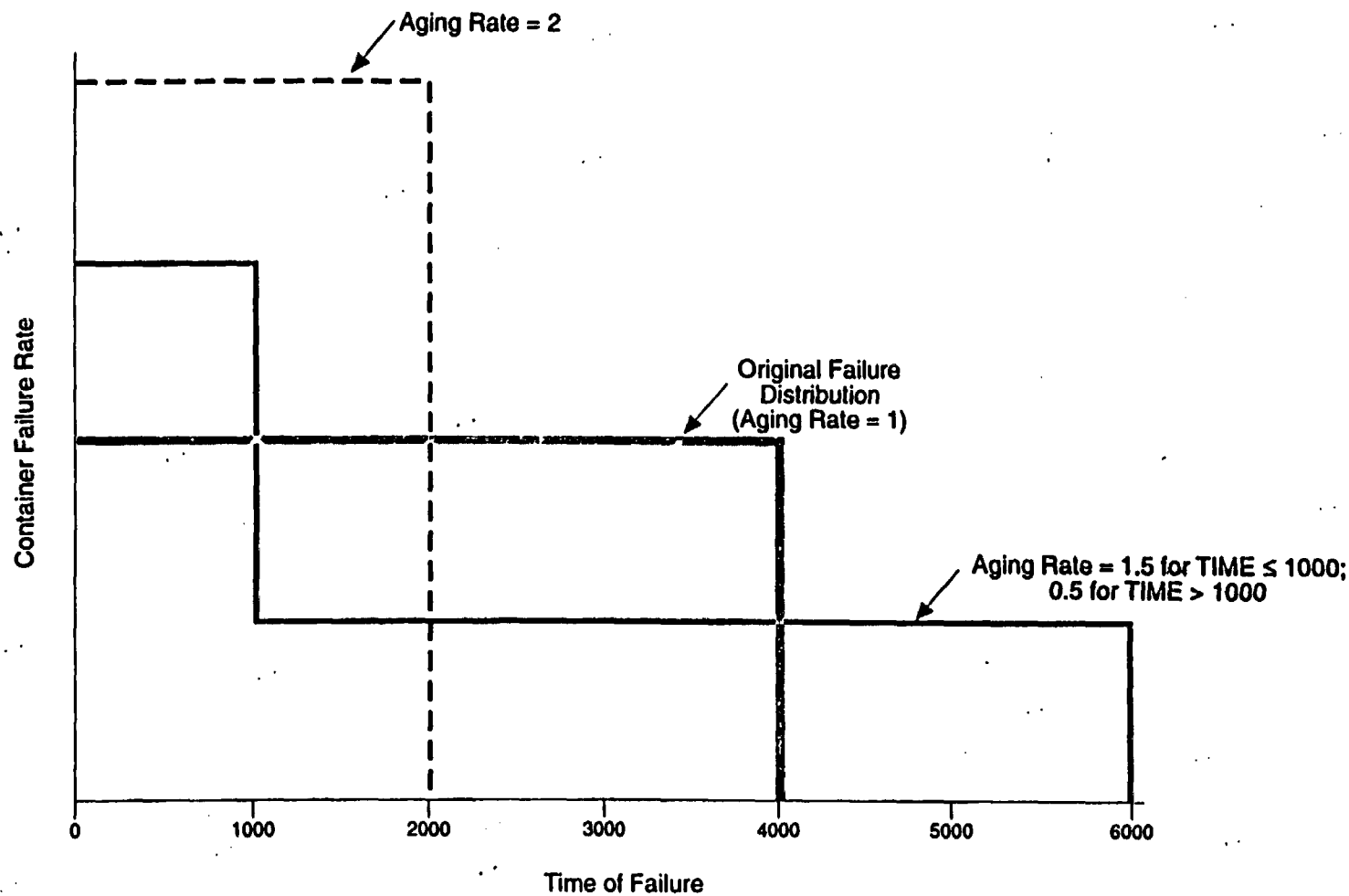


FIGURE **10-5**
**EFFECT OF AGING RATES**

PROJECT NO. 973 1805.001 DRAWING NO. 73357 DATE 6/20/97 DRAWN BY EA

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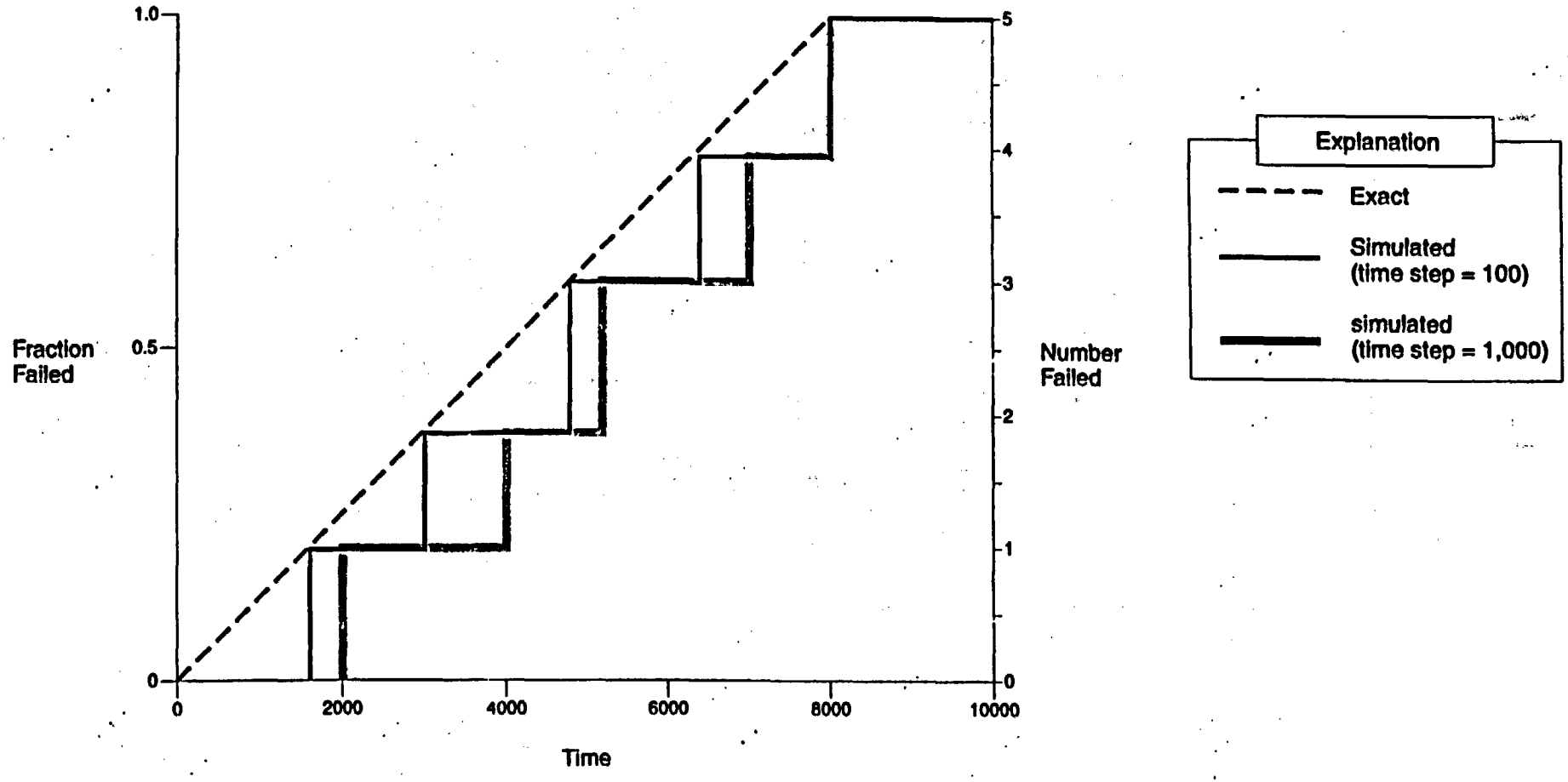


FIGURE 10-7
DISCRETIZATION OF PRIMARY CONTAINER FAILURE

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# Computing the Free Exposure Rate

- $e_i(n,t) = e_{i,f}(n,t) + e_{i,g}(n,t) + e_{i,b}(n,t)$

  $e_{i,f}(n,t) = NWP_i \; I_f(n,t) \; c(t)$

- where

  $NWP_i$ = number of waste packages in group i

  $I_f(n,t)$ = free inventory of RN n at time t in a single WP (M/cont)

  $c(t)$ = primary container failure rate (1/t)



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# Computing the Gap Exposure Rate

- $e_i(n,t) = e_{i,f}(n,t) + \underline{e_{i,g}(n,t)} + e_{i,b}(n,t)$

$$e_{i,g}(n,t) = NWP_i \, I_g(n,t) \, g(t)$$

- where

$NWP_i$ = number of waste packages in group i

$I_g(n,t)$ = gap inventory of RN n at time t in a single WP (M/cont)

$g(t)$ = rate at which matrix becomes unprotected (1/t)



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# Computing the Gap Exposure Rate (cont)

$$g(t) = \int_0^t [c(t)\, w(\tau,t) + c(\tau)\, w(t,\tau)]\, d\tau$$

- where

  w(t1,t2) = secondary container failure rate at time t1 for a primary container which has failed at time t2 (1/t)



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# Computing the Bound Exposure Rate

- $e_i(n,t) = e_{i,f}(n,t) + e_{i,g}(n,t) + \underline{e_{i,b}(n,t)}$

$$e_{i,b}(n,t) = N_c\, M_{uu,i}(t)\, k_{a/d}\, I_b(n,t)$$

- where

$I_b(n,t)$ = bound inventory of RN n at time t in a single WP (M/cont)

$M_{uu,i}(t)$ = fraction of unprotected, unaltered/undissolved waste matrix in group i at time t

$k_{a/d}$ = waste matrix alteration/dissolution rate (1/t)



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# Computing the Bound Exposure Rate (cont)

- $M_{uu,i}(t)$ is calculated based on the following differential equation:

$$\frac{dM_{uu,i}}{dt} = g(t) - M_{uu,i}(t)\, k_{a/d}$$

- solved as:

$$M_{uu,i}(t) = \frac{M_{uu}(t-\Delta t) + g(t)\Delta t}{1 + k_{a/d}(t)\Delta t}$$

- original timestep subdivided by 4



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# Matrix Degradation Rates

- **Specified as fractional rates (1/yr)**
- **Must be carefully defined**
- **Issues:**
  - Actual degradation is typically a function of surface area ($g/m^2/yr$)
  - Fractional rate = absolute rate times specific area ($m^2/g$)
  - for most geometries, specific area increases with time
  - For many materials, absolute degradation rate decreases with time



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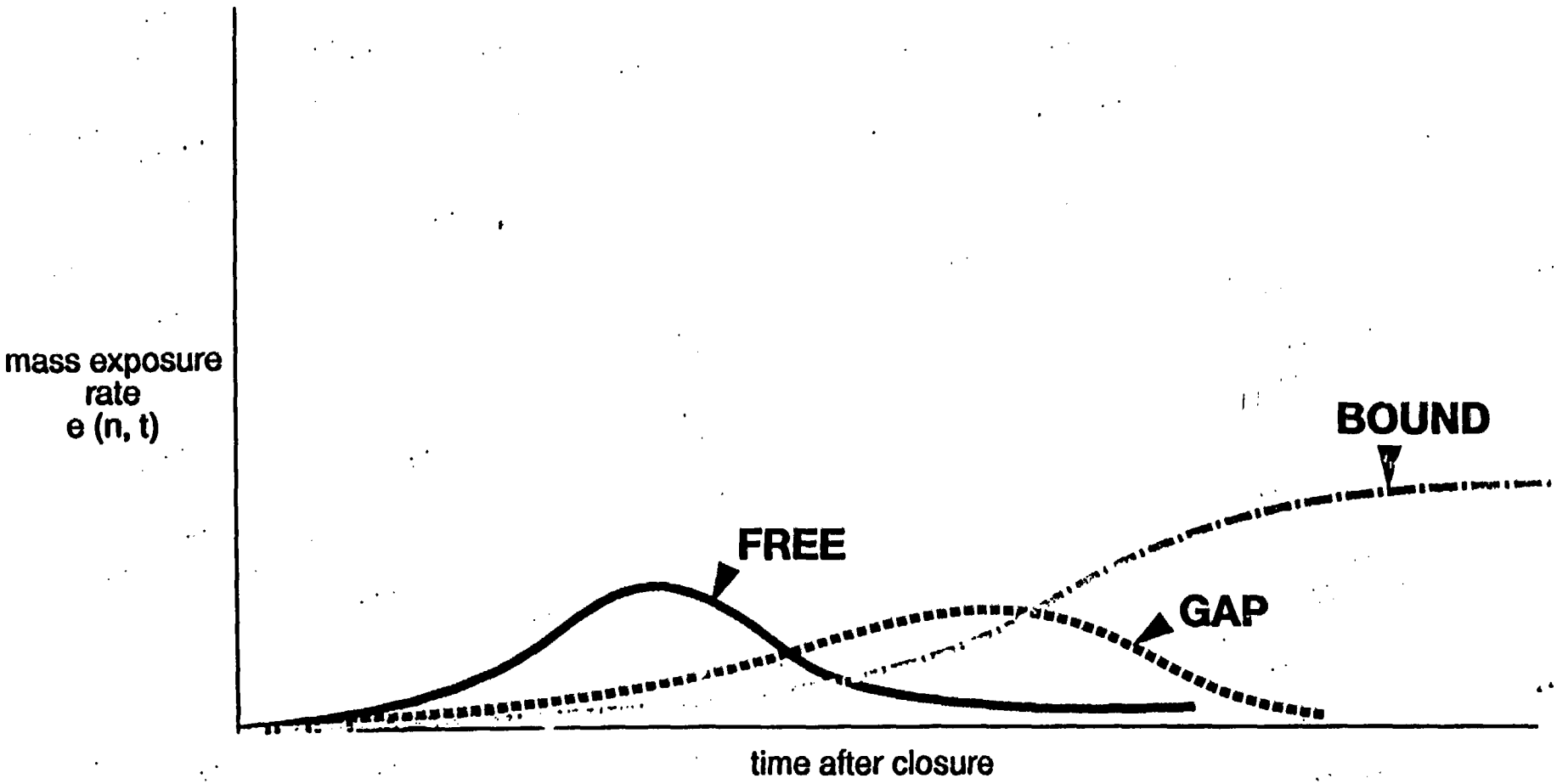
# Radionuclide Exposure Distribution

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# Mass Transport Within and Away from Source

- RIP associates one or more cell pathways with the source
- The associated cells are defined to represent the behavior of a single container in the source
- RIP scales some properties of these pathways with the number of failed primary containers
  - volumes
  - diffusive areas
  - flow rates



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# Implications of Simulating Groups of Containers

- Implicit assumption is that all exposed mass is evenly distributed among failed containers
- Likely to be conservative (solubility constraints)
- To simulate more accurately, would need to assign cells to every container

# Representing Spatial Variability

- **Variable parameters can take on different values depending on where they are referenced in RIP**
- **User can define specific environments**
  - An environment is a set of values of specified variable parameters
- **User assigns specific environments to various locations (pathways and sources) in RIP**
- **RIP automatically uses the value of the variable parameters which are appropriate for the particular location being referenced in a calculation**

# Assigning Environments

- **A single environment can be assigned to any given pathway**
- **Since sources represent a collection of objects (containers), multiple environments can be assigned to a source**
  - User specifies the fraction of containers in each environment

# Source Term Groups

- **A source term group is defined by a particular source/environment combination**
- **Source term calculations are performed separately for each source term group**
  - RIP internally creates "clones" of all associated cells for a source which has multiple groups
  - These are denoted CELLc1, CELLc2, ...
- **Results can be reported by source term group and by cloned cell**



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# Receptor Model

- **User must specify:**
  - specific receptors
  - exposure routes; and
  - conversion factors
- **An exposure route is defined by associating a conversion factor for a specific receptor with the concentration of the species in a medium within a specific pathway**
- **Multiple receptors, exposure routes and conversion tables can be defined**



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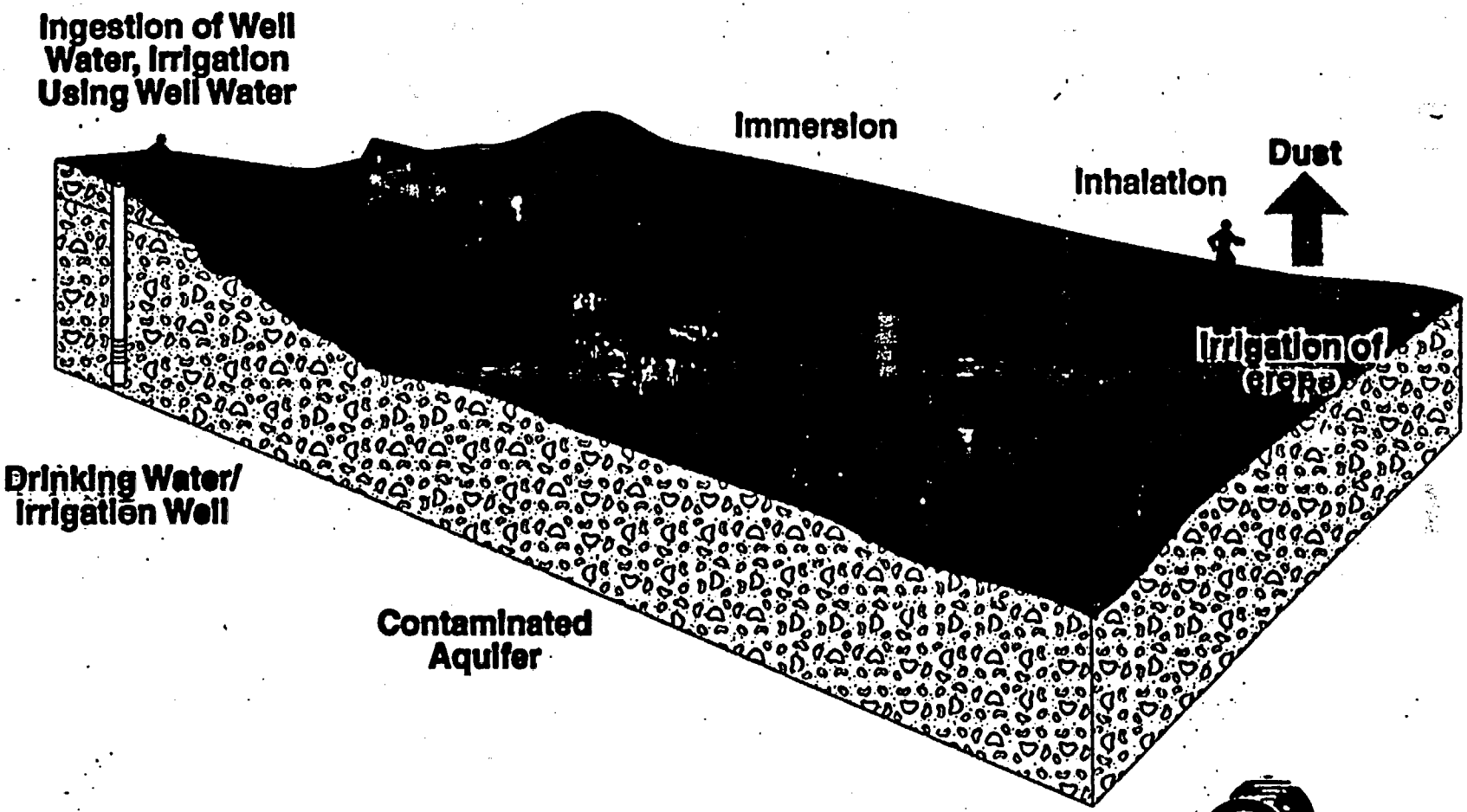
# Example Biosphere Model



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# Computing an Impact

$$D_k = R_k \sum_{\substack{\text{all} \\ \text{routes, r}}} \sum_{\substack{\text{all} \\ \text{species, s}}} F_{krs} C_{rs}$$

**where:**

$D_k$ is the impact to receptor k [mrem/yr]

$R_k$ is the risk conversion factor for receptor k [$mrem^{-1}$]

$F_{krs}$ is the conversion factor for species s in media associated with route r for receptor k [(mrem/yr)($g/m^3$)]

$C_{rs}$ is the concentration of species s in media associated with route r [$g/m^3$]



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# Conversion Factors

- Conversion factors are impacts associated with a unit concentration
- For example, for doses associated with concentrations in a fluid medium, they have units of (mrem/yr)/(g/m$^3$)
- Typically computed within a spreadsheet and imported into RIP



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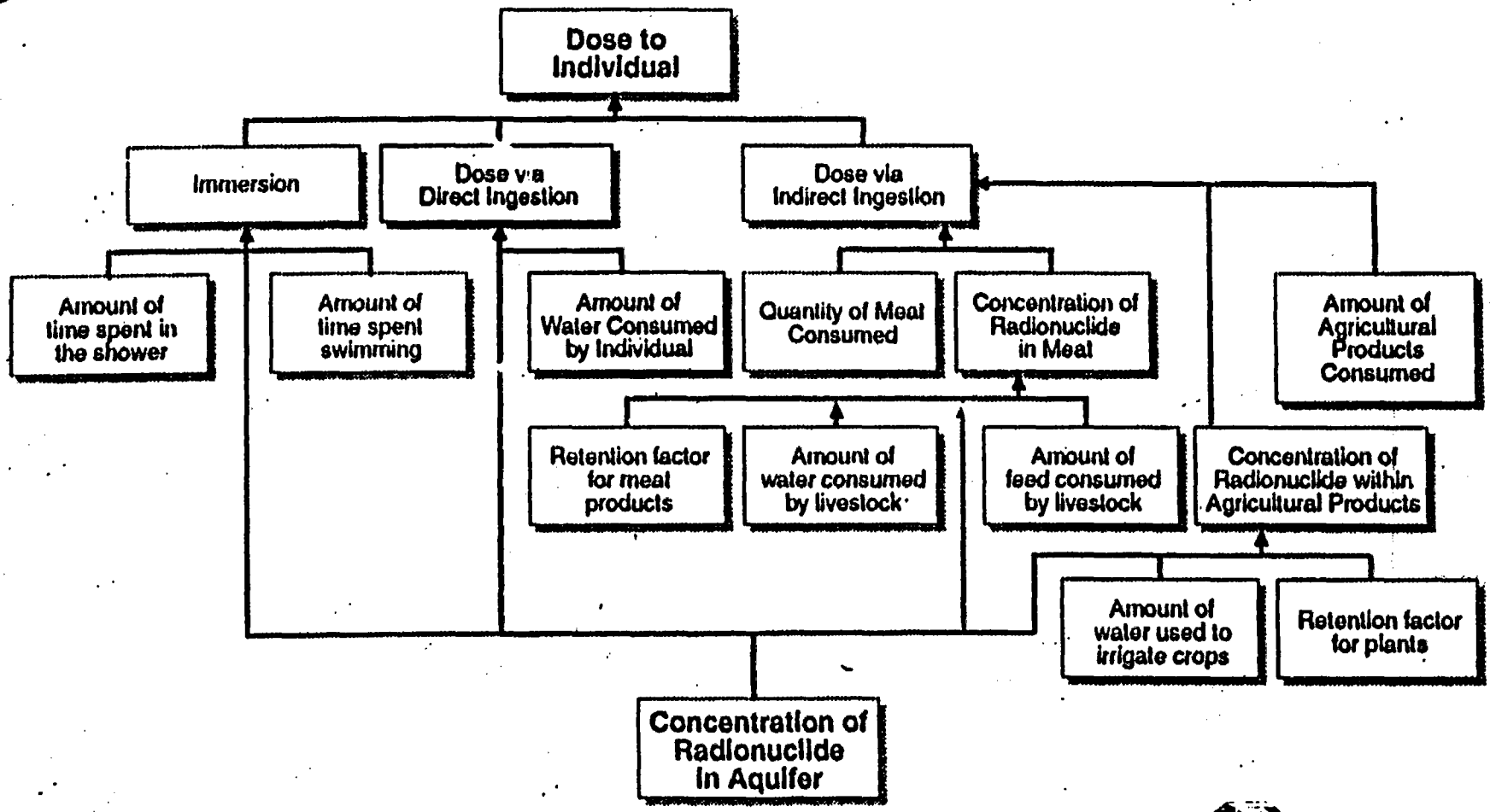
# Influence Diagram for Dose

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# Disruptive Events Model

- **Define a set of significant events**
- **Describe each event probabilistically**
  - rate of occurrence
  - descriptors
- **Describe consequences of event**
  - probabilistically
  - function of descriptors



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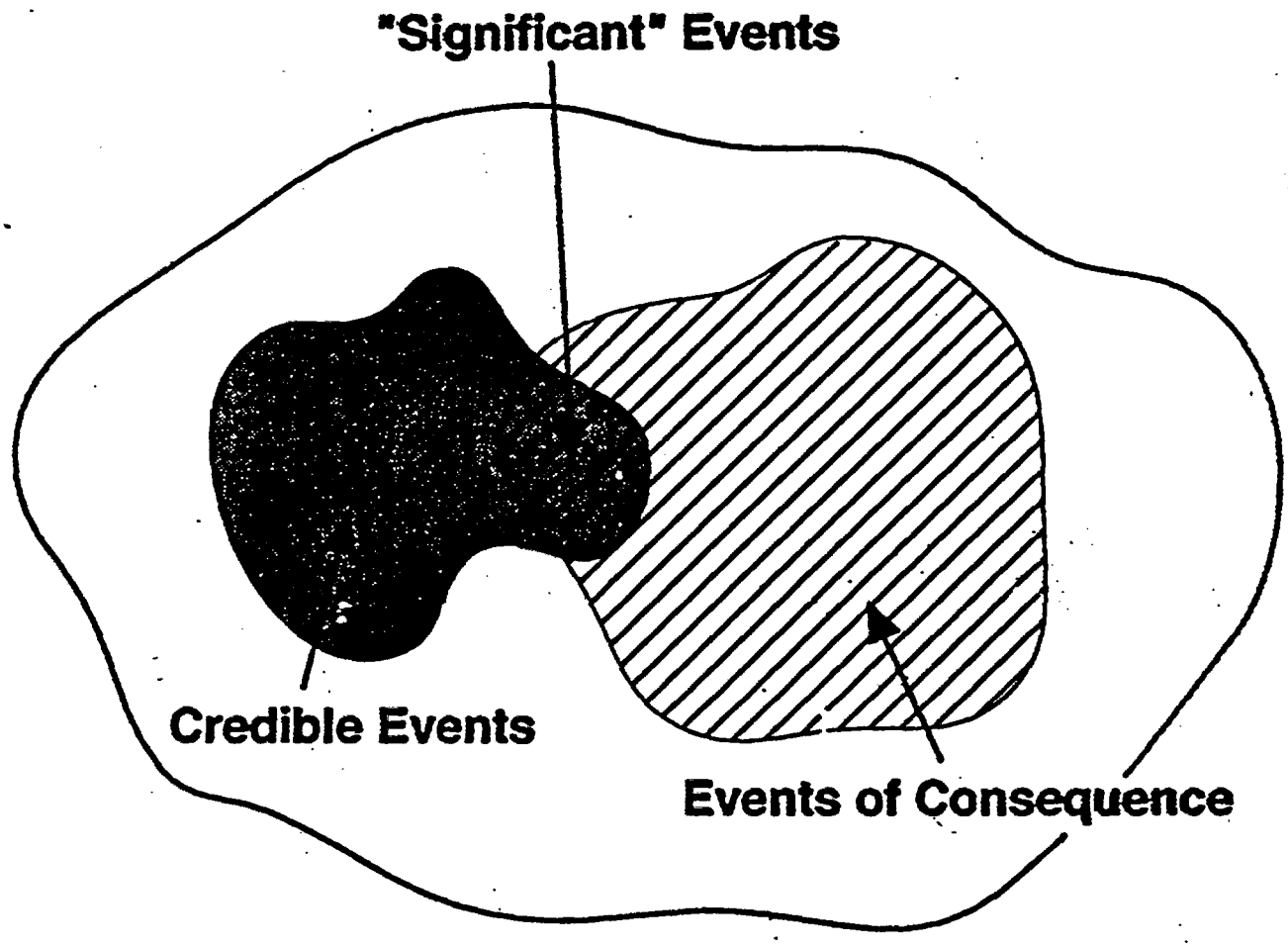
# Set of All Conceivable Disruptive Events

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# Event Occurrence

- **Three types of events:**
  - regularly occurring
  - Poisson
  - conditional
- **Event can be specified to reoccur or occur only once**
- **Each event can have descriptor parameters which are re-realized when event occurs**

# Event Consequences

- **Disrupt containers**
- **Move containers to a pathway**
- **Move portion of mass in a pathway to other pathways**
- **Modify parameters**
  - can be conditional
  - add, replace, or multiply

# Post-Processing

- **Graphical Display**
  - Distribution of result
  - Time history of result or particular parameters
  - Scatter plots of parameters vs. results
- **Correlation analysis**
- **Raw data display**
- **Export output to standard statistical analysis packages**



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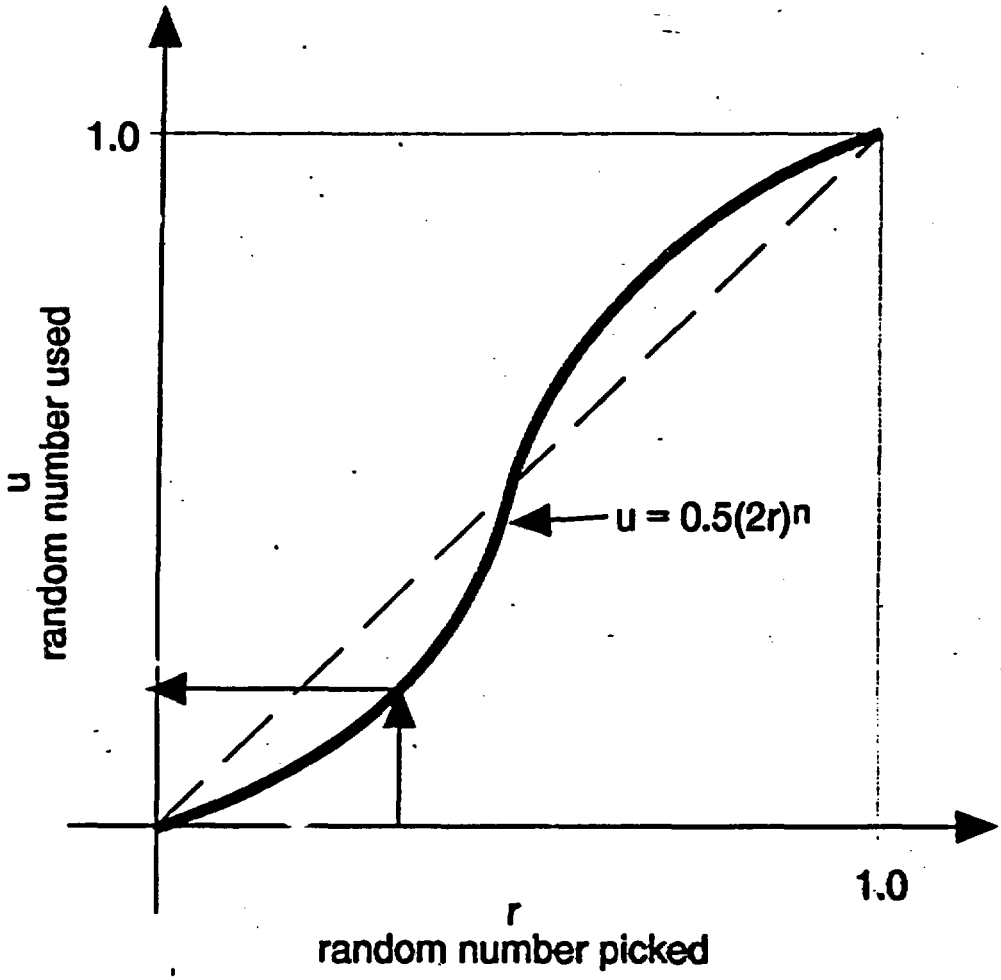
# Post Processing

- Allows Real-time viewing of complex data
- Create sub-sets of results
  - Screen by result
    - only consider realizations where threshold release is exceeded
  - Screen by input parameter
    - only consider realizations where earthquakes occur
  - Screen by result and input parameters
    - only consider realizations where earthquake occurs *and* threshold release is exceeded

# MONTE CARLO SAMPLING DETAILS

- Repeat Sampling Sequence
- Latin Hypercube Sampling
- Importance Sampling
  - for parameters
  - for events

# Parameter Importance - Sampling Algorithm

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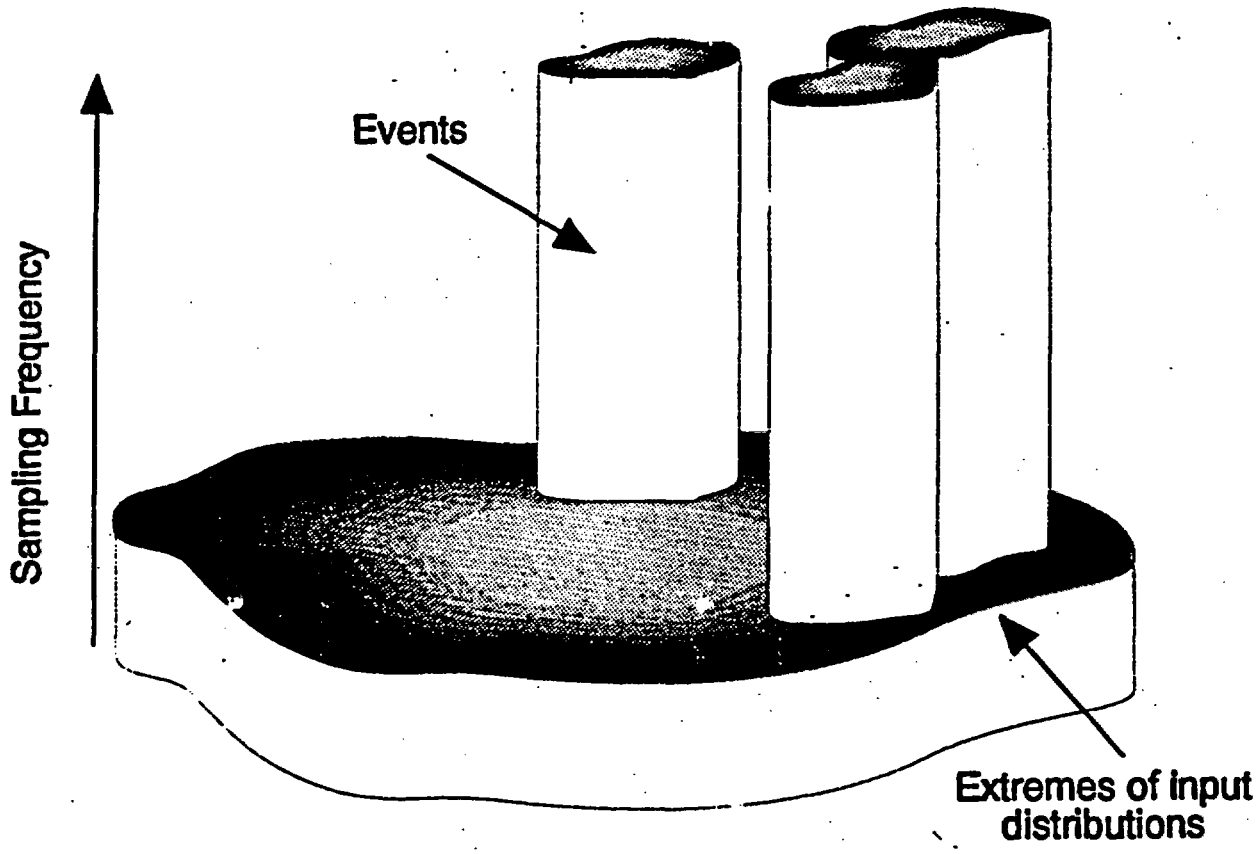
# Importance Sampling of Parameters and Events




Bias towards realizations in which events occur, and realizations at the extremes of the input distribution

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