U.S. DEPARTMENT OF ENERGY
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

NUCLEAR WASTE TECHNICAL REVIEW BOARD
FULL BOARD MEETING

SUBJECT: COMBINING PROCESSES: AN ENGINEERED BARRIER SYSTEM SOURCE TERM

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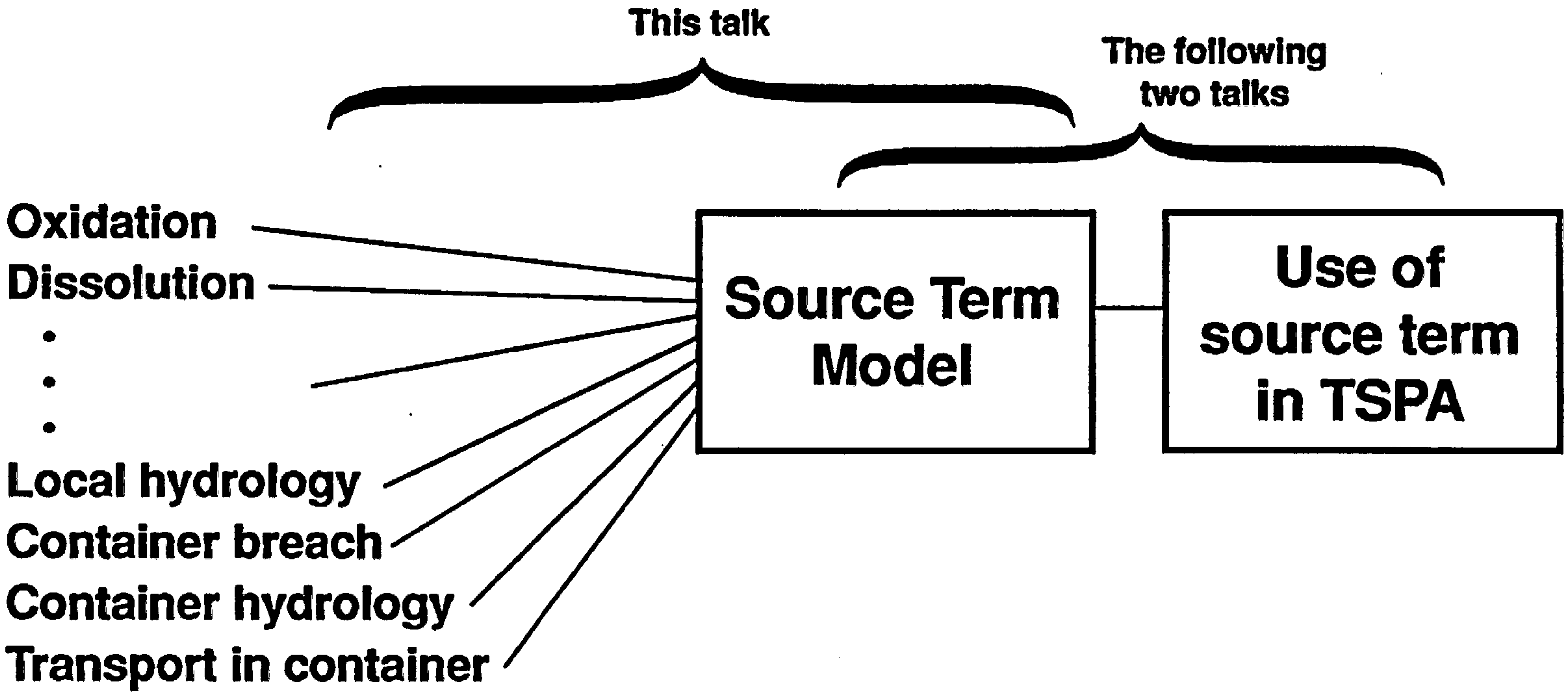
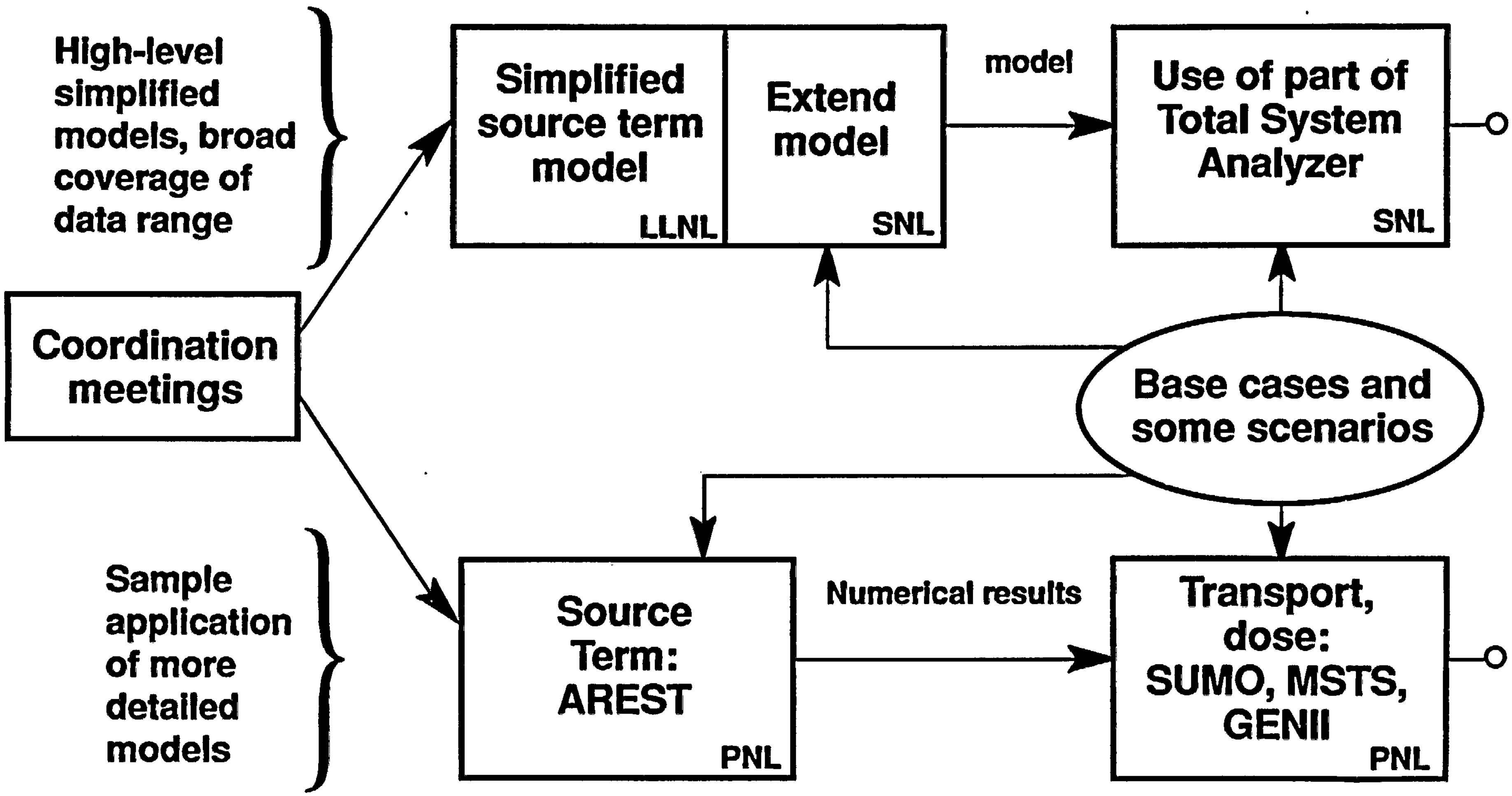
This Morning's Talks by DOE Contractors Focus on the Use of the Detailed Models and Data in Systems-Level Applications

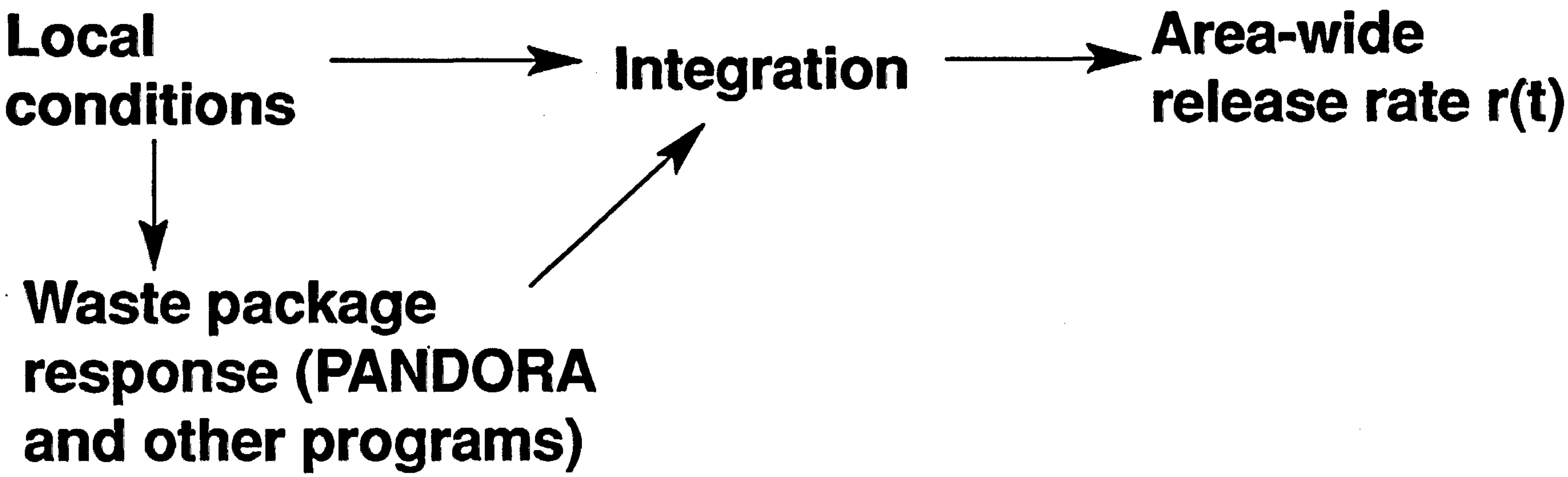


Two Trains of Analyses were Carried out in DOE's TSPA-91 for Complementary Purposes



- Today's talks by LLNL, PNL, and SNL focus on the source term

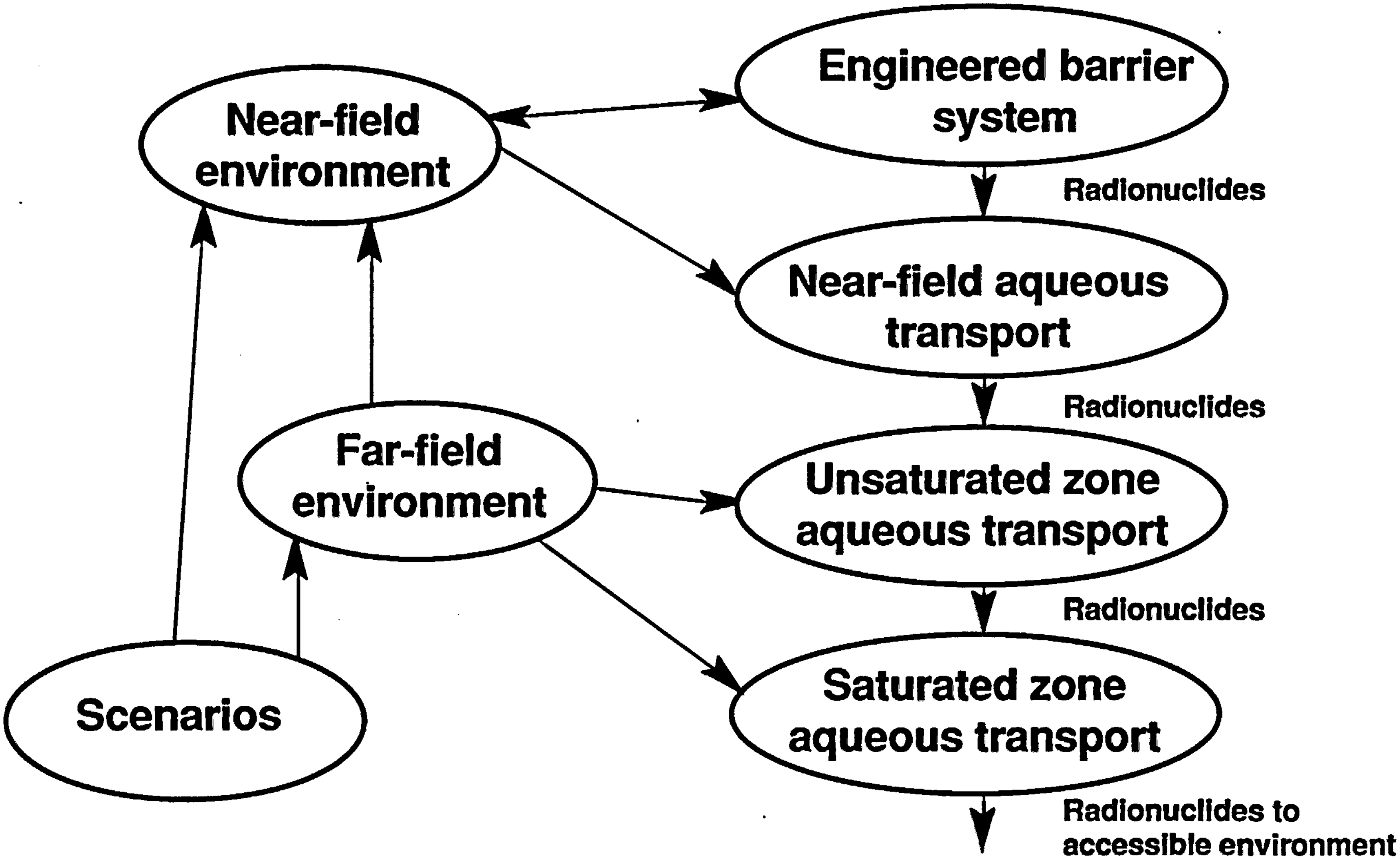
A Source Term Requires Single-Package Behavior and Integration over Packages



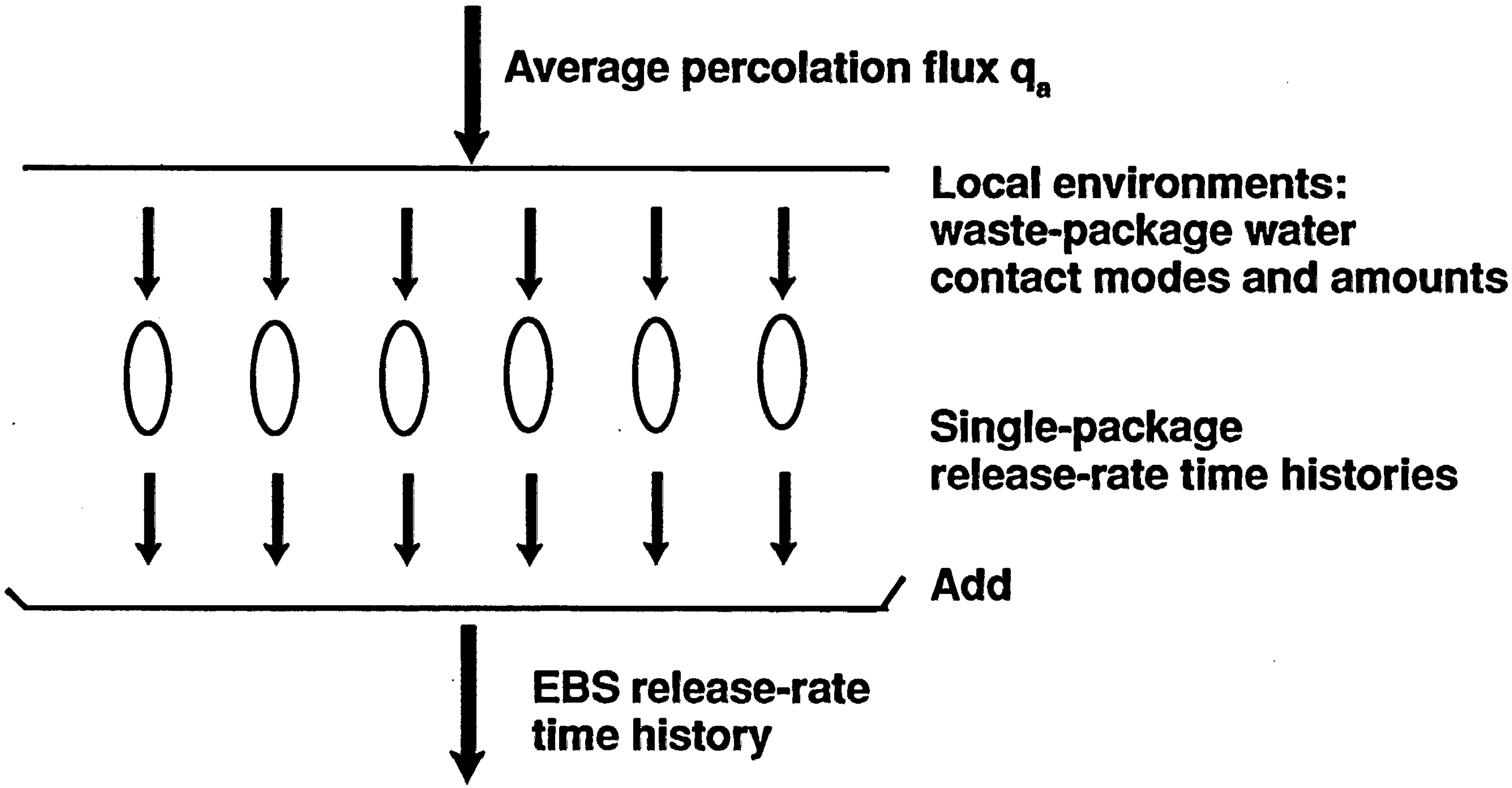
Desired Features of a SourceTerm for Total System Performance Assessment (TSPA)

- Simple
- Has the major features of the process results
- Applicable over a wide range of parameter values
- Uses the total system parameters, where appropriate (q_a, q_o)
  - Percolation flux (q_a)
  - Saturated hydraulic conductivity of porous rock matrix (q_o)

Subsystems Act as Boundary Conditions and/ or Barriers in the Base-Case Aqueous Release



At the Core of the Engineered Barrier System (EBS) are Single Waste Packages with Different Local Environments



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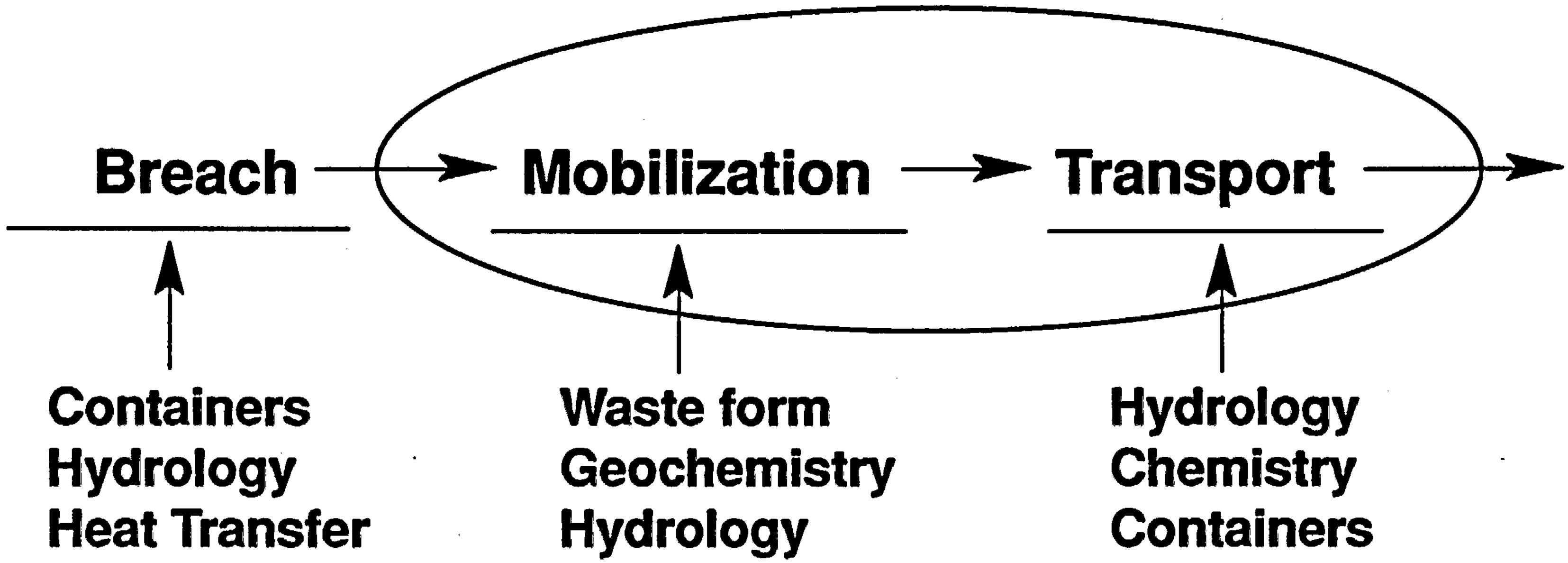
Some Issues in the Source-Term Modeling Process

- Linking of processes
  - On single waste packages
  - On area-wide set of waste packages
- Areal averages/localized variations
- Correlations
  - Among inputs
  - Of outputs with inputs

For Single Waste-Package Response, the PACE-90 Working Group 2 Focused on the Processes Near the End of the Causal Chain



Earlier processes are treated by input data structures

Within a Single Waste Package or a Set, Multiple Alternatives Must be Modeled

EBS transport processes

- Diffusion
- Flow-through
- Bathtub
- Gaseous only

x

Radionuclide chemical types

- High solubility ✓
- Low solubility ✓
- Gas (not included)

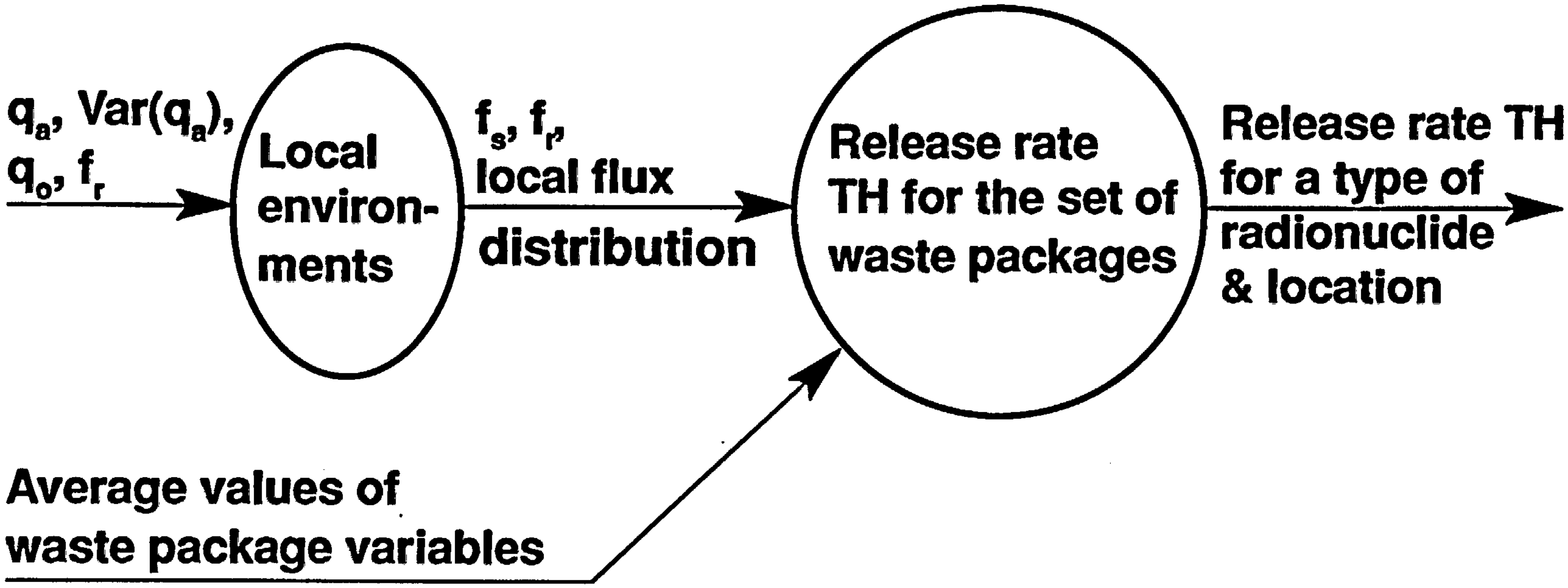
x

Source location properties

- Rapidly accessible location (cladding surface, cladding gap)
- Matrix location

For each important alternative, an area-integrated result was calculated

First the Distribution Was Determined of Local Environments for the Release Rate Processes



TH: Time history
q_a: Average percolation flux
Var(q_a): Spatial variance of q_a
q_o: Saturated hydraulic conductivity of the porous rock
f_s: Fraction of boreholes with seepage flow
f_r: Fraction of boreholes with rubble

Areal Averages ⟶ Localized Variations

- The simplified source term for TSPA-91 treated local-environment variability in
  - Hydrology
  - Rock mechanics (for a diffusion pathway)
  - Container breach times

- Within a waste package, a fraction of the spent fuel is wet at any time. The simplified model assumed this fraction is a constant

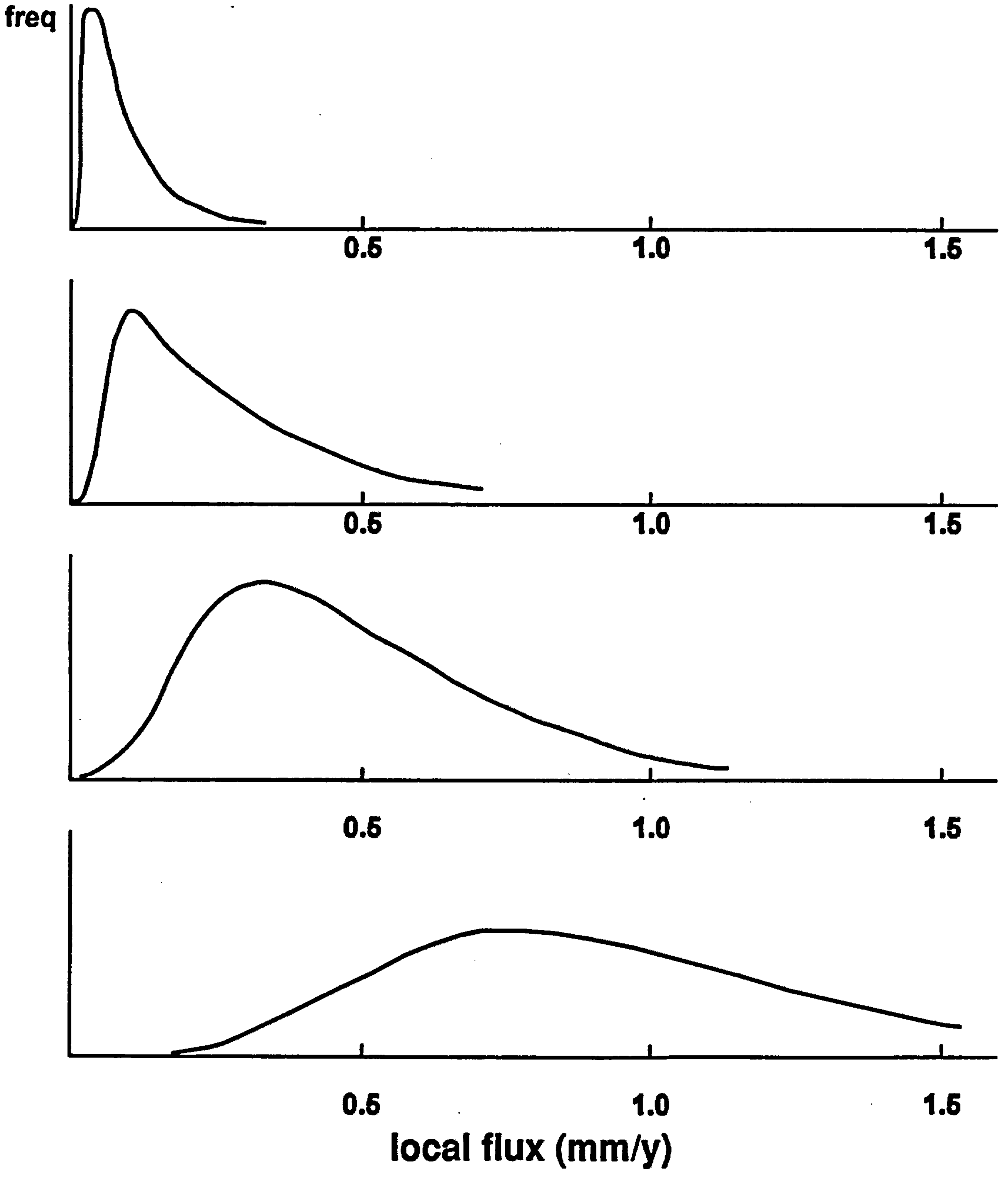
Some Specific Features of the Mountain-Wide Base Case Hydrology for TSPA-91

- The probability distribution of average percolation flux covers a wide range (0 mm/y - 7 mm/y and up)
- As average flux increases, the local environments are expected to change:
  - More waste packages get wet
  - The advective flux at wet packages increases
- The average percolation flux influences both the source term and the far-field transport
- Does the source term change smoothly or as a step function versus the average percolation flux?

Some Features of the Local-Environments Model

- For a waste package to have water contact, it requires rubble in the borehole, or seeping water, or both
- Local percolation flux is lognormally distributed, with repository-wide average equal to the average percolation flux
- Local seepage or fracture flow occurs if the local water flux exceeds the saturated hydraulic conductivity of the matrix
- Rubble and seepage occurrence are independent
- The effective diffusion coefficient in the rubble depends on whether seepage is present

As the Average Percolation Flux Increases, a Greater Fraction of the Waste Packages Experience the Larger Local Percolation Flux Values



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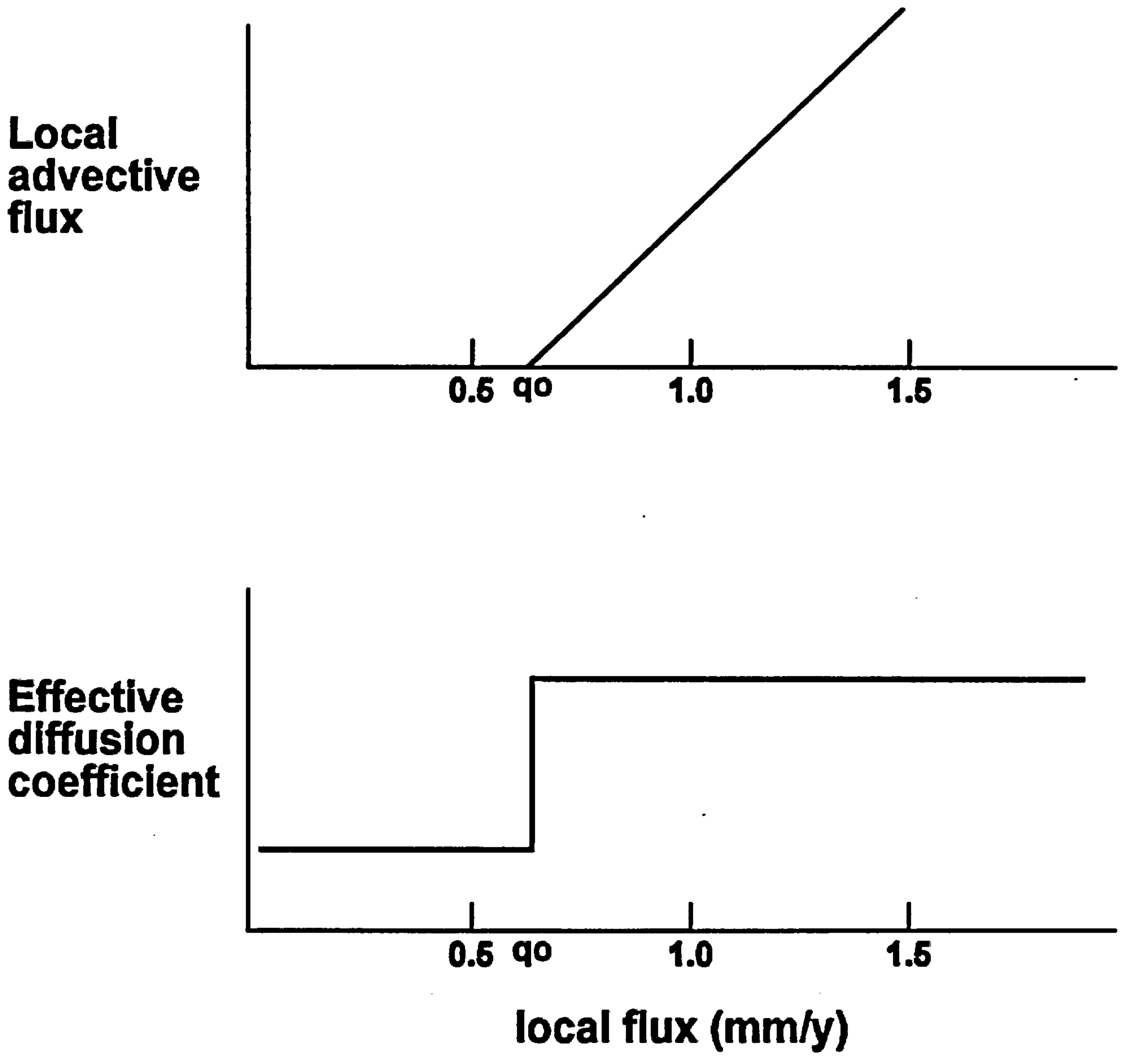
As the Local Percolation Flux Goes Up, the Local Advective Flux and the Effective Diffusion Coefficient Change



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Output of the Model: A Distribution of Local Environments

f_r: Fraction of waste-package boreholes with rubble

f_s: Fraction of waste-package boreholes with seepage

Fraction of waste package	Type of water contact mode
$f_s \cdot (1 - f_r)$	Advective, with a distribution of local water flux
$(1 - f_s) \cdot f_r$	Diffusive with low diffusion coefficient
$f_s \cdot f_r$	Combined advective and diffusive with higher diffusion coefficient
$(1 - f_s) \cdot (1 - f_r)$	None

Geochemistry Variation is a Fertile Field for Future Modeling

- Local variability in geochemistry was not treated
- Within a waste package, the chemistry will be dependent on the hydrology, specifically on the following:

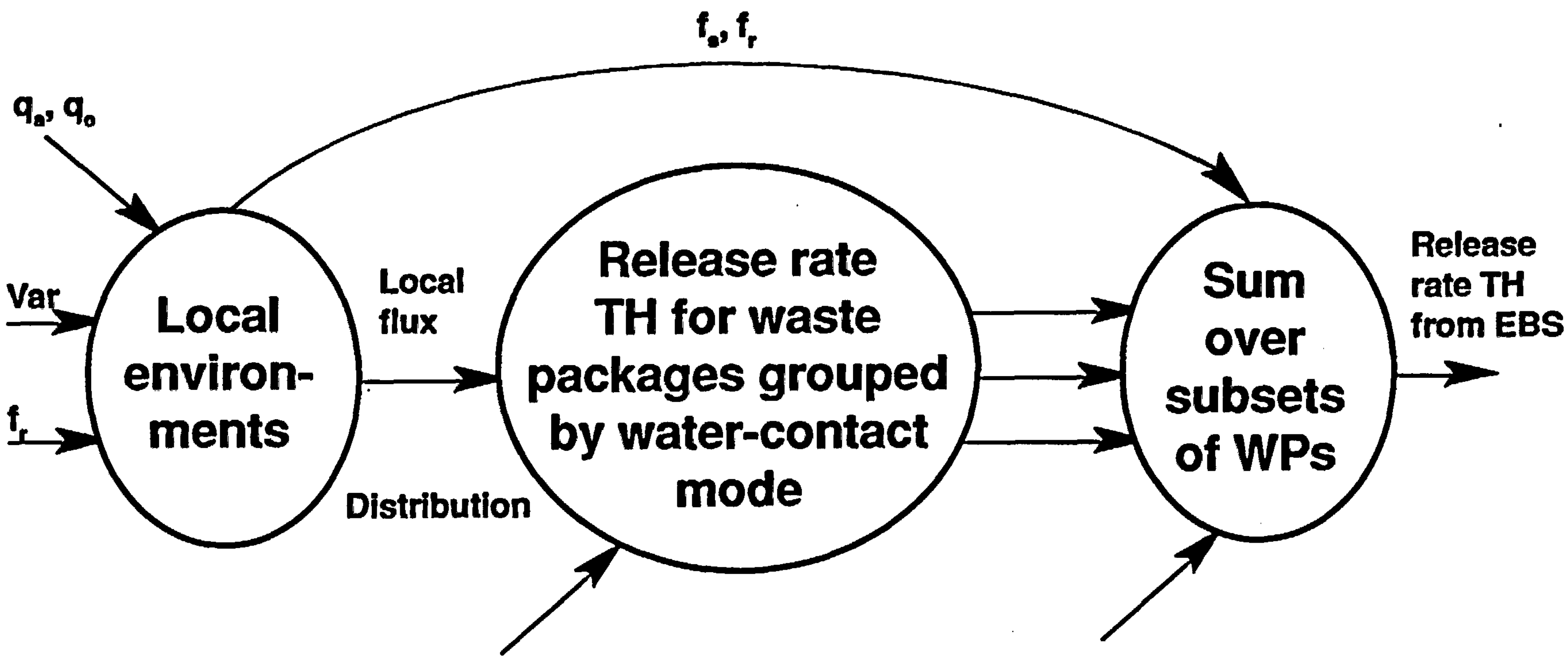
$$\frac{\text{Moles Ca /y}}{\text{Moles U reacted /y}} = \frac{\text{Water influx/y x Conc. of Ca}}{\text{Bulk Surface wet} \times \dfrac{\text{Grain surface}}{\text{Bulk surface}} \times \text{Reaction rate}}$$

↑ doesn't seem to be appropriate

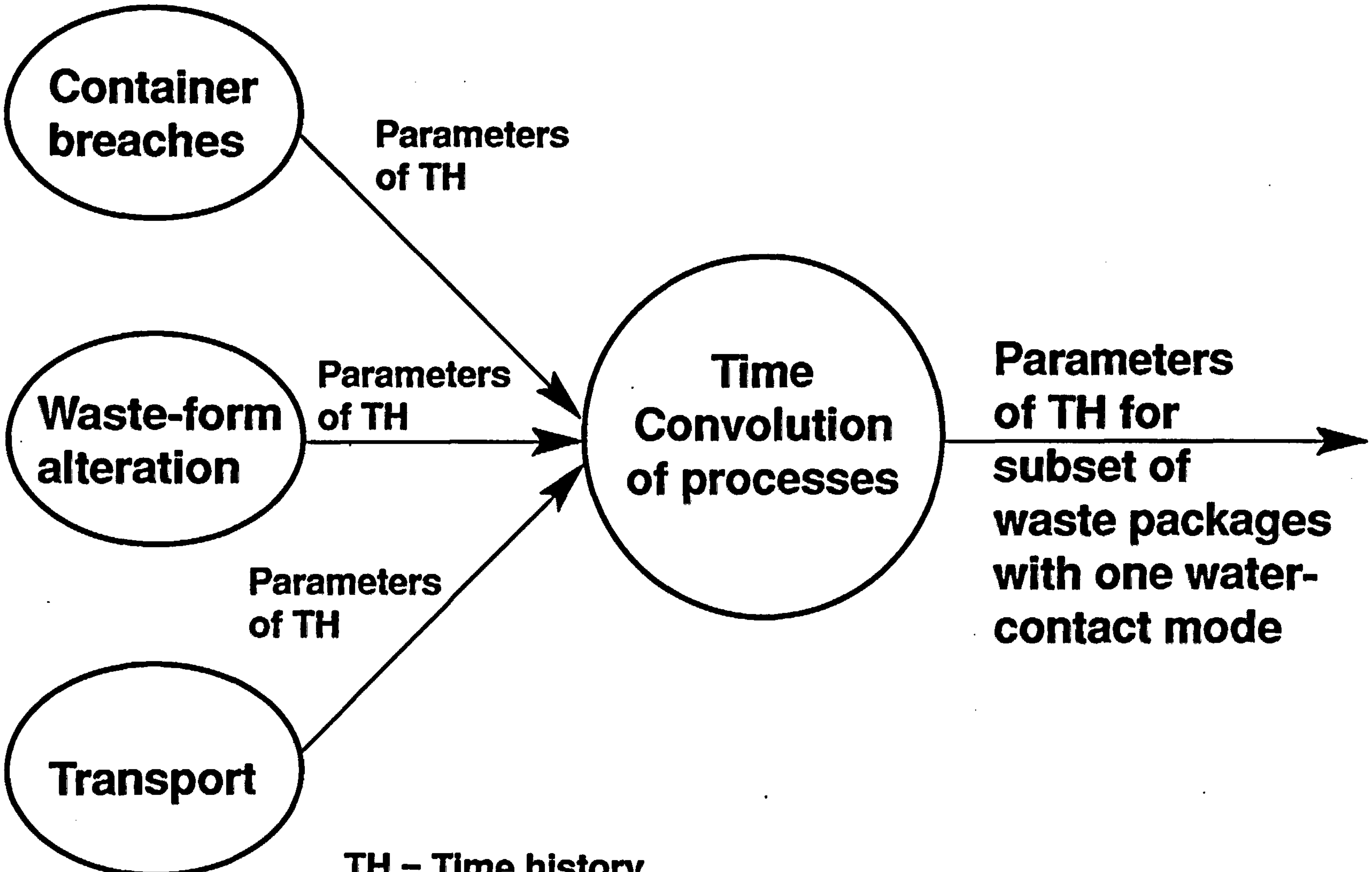
Organization of the Release Rate Calculation

- Top level
  - Radionuclide type
- Second level
  - Radionuclide location
- Third level
  - Water contact/transport mode
    * Diffusive moist
    * Diffusive wet plus advective in parallel
    * Advective, no diffusion
    * No liquid pathway

The Release-Rate Calculation is Grouped by Water-Contact mode



For Each Water-Contact Mode, the Release Rate TH Depends on Containers, on Waste Form/Geochemistry, and on Hydrology/Transport

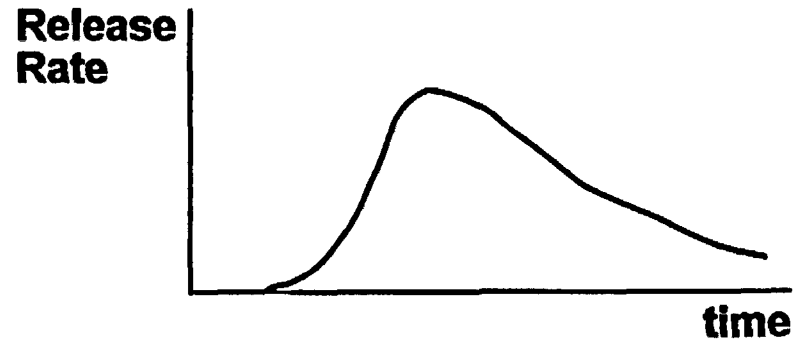


TH = Time history

Earlier Work Found the Release-Rate Curves Had a Few Key Characteristics

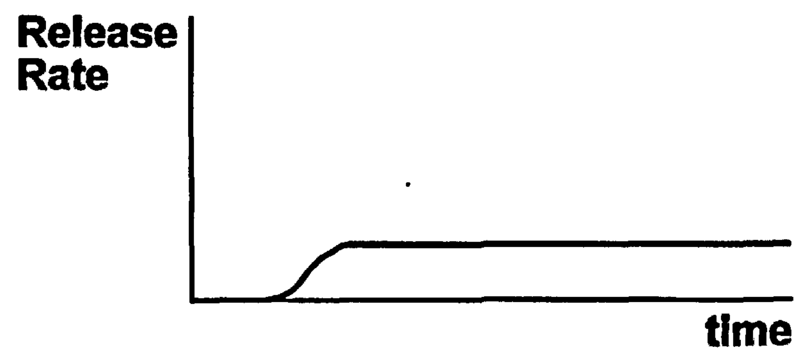
For high-solubility radionuclides:

- Limited duration
- Peak value ~ 1 / duration



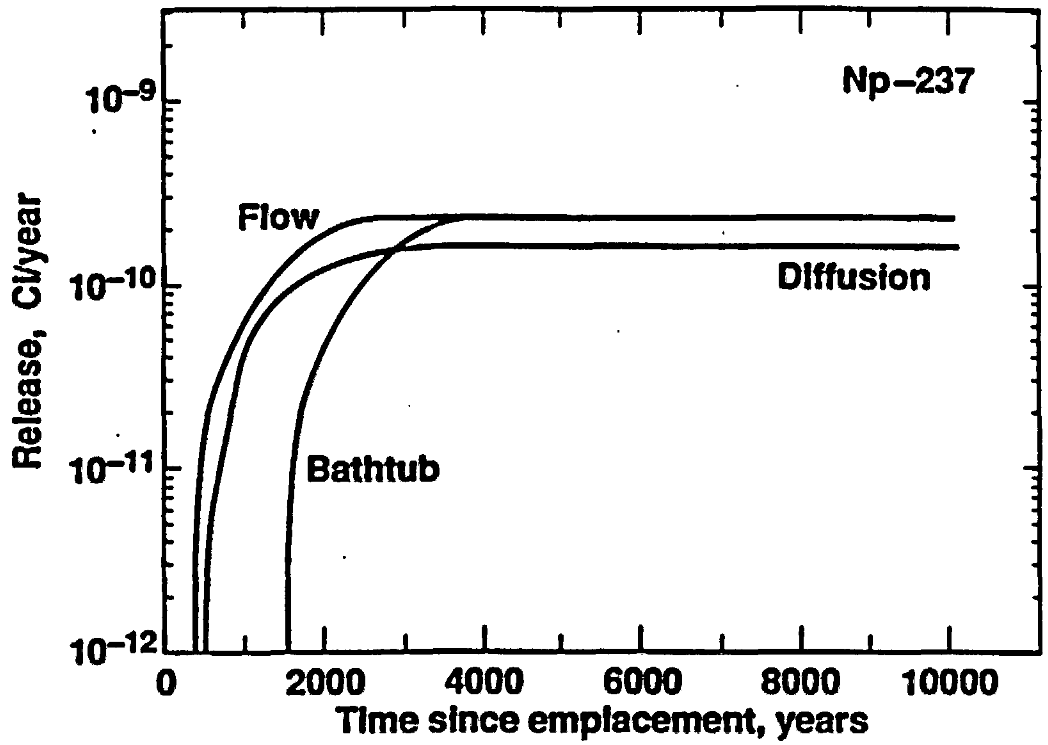
For low-solubility radionuclides:

- Very long duration
- Constant plateau value

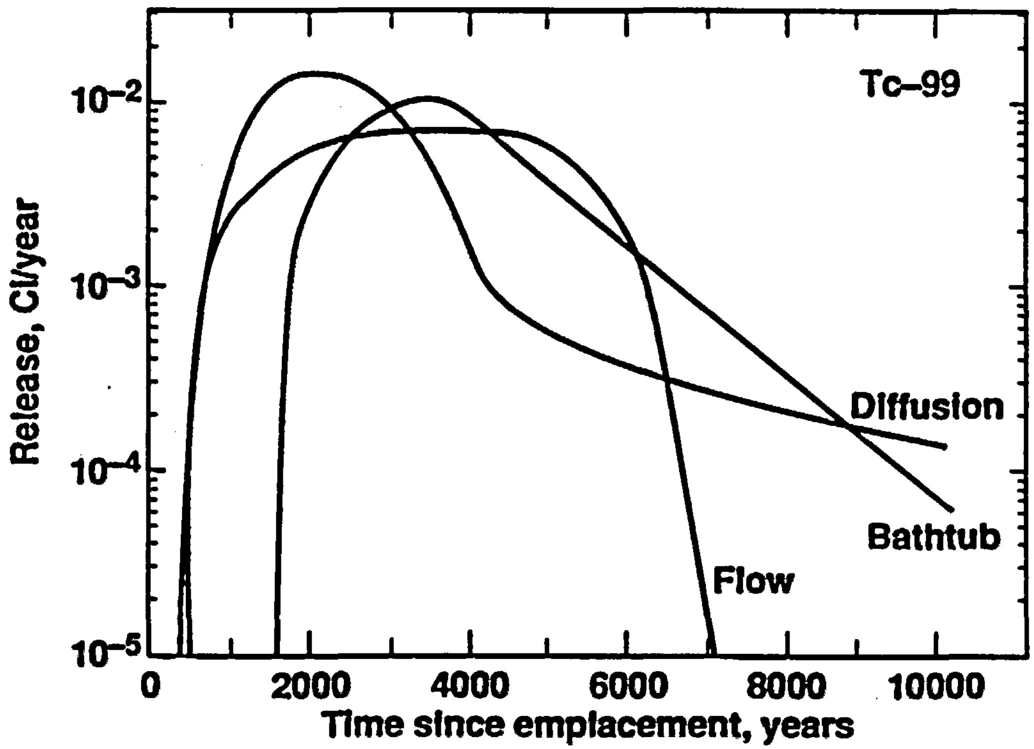


The simplified source-term model will calculate key parameters of the output curves.

Release of Low-Solubility Np-237 was of Low Amplitude, Long Duration

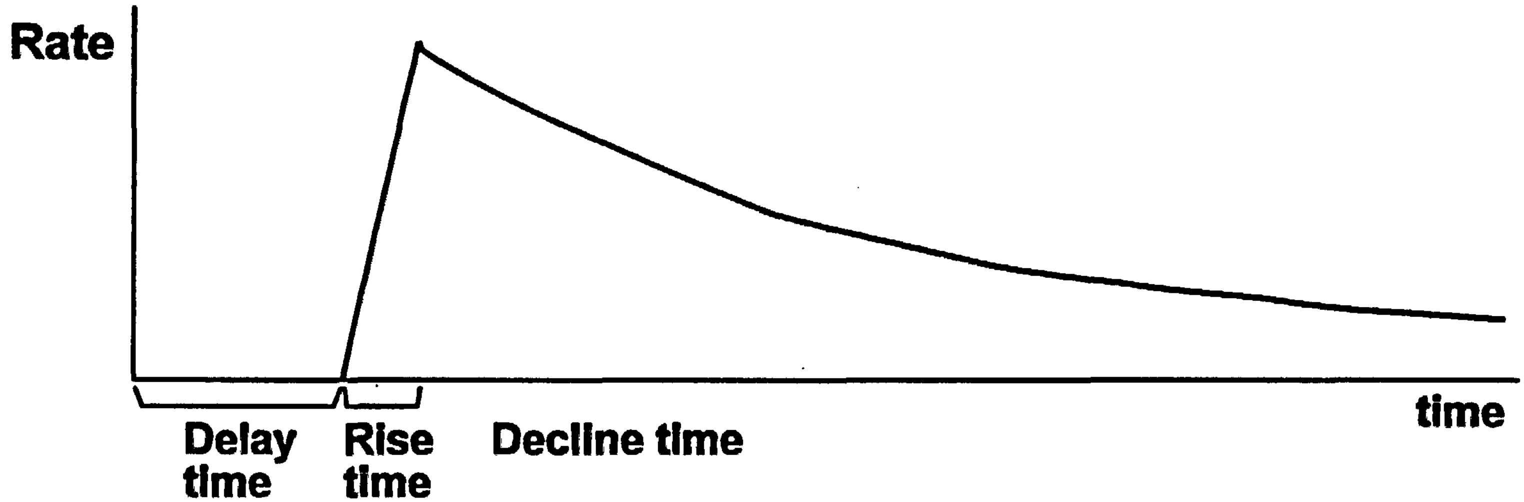


Release of Tc-99 from Wet Waste Packages was of Relatively Short Duration and High Amplitude



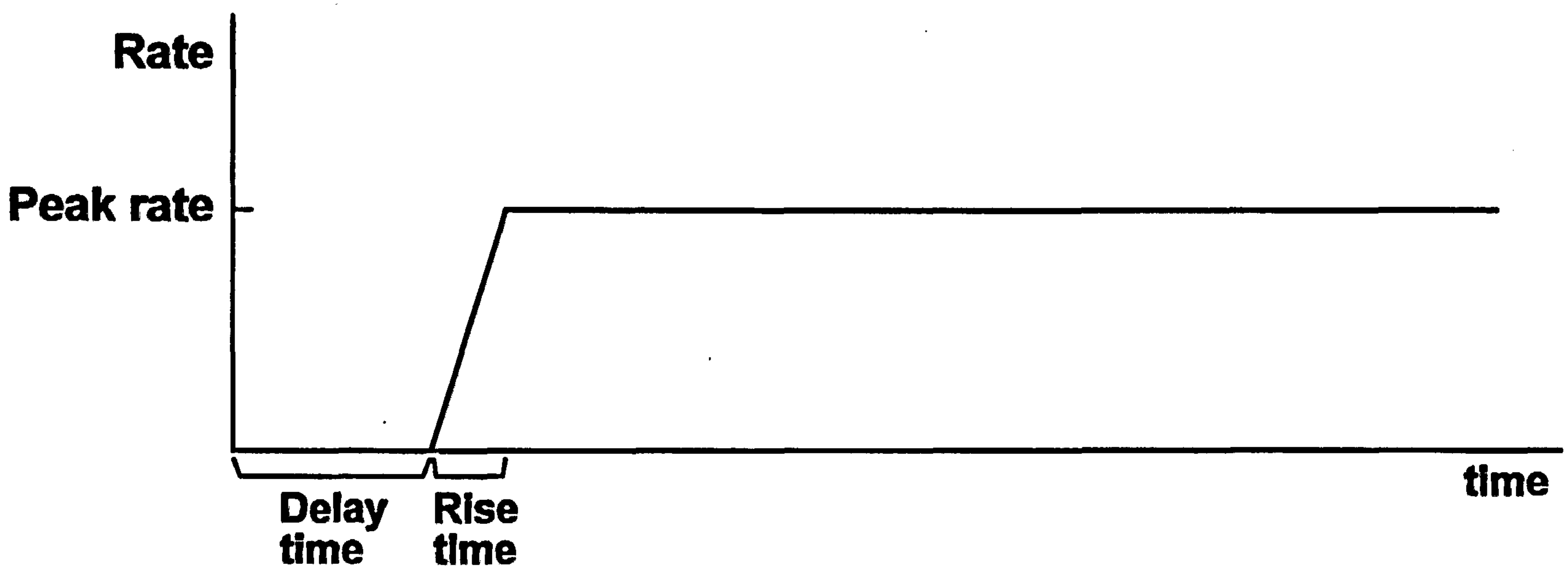
For Simplicity and for Focus on the First-Order Effects, Assumed a Generic Shape of the Time Histories

For highly soluble radionuclides:



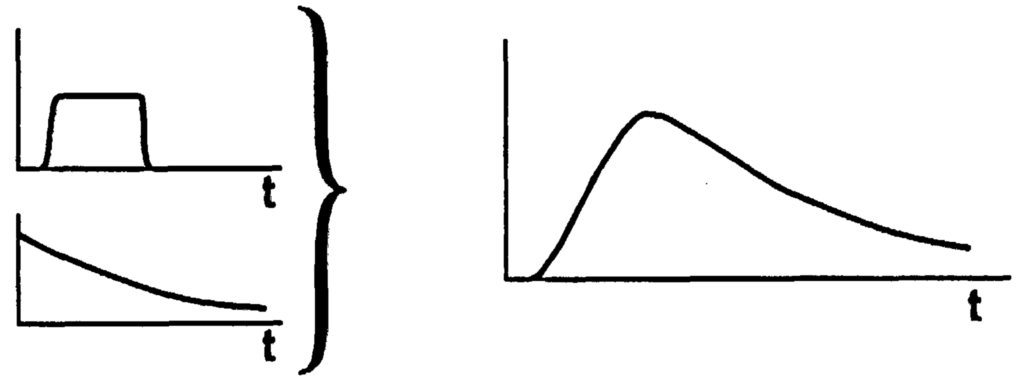
- Generic shape -- main effects only
- Parameters guided by sensitivity analysis
- Assume a time convolution gives same shape, new parameters

Shape for Solubility-Limited Radionuclides

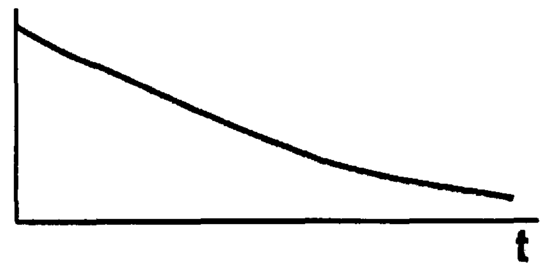


At the Center of the Release Model are the Single-Process Time Constants

Container breaches:
Time spread in wetting
Time spread in breaches after becoming wet



Waste form alteration:
Characteristic time = 1 / Rate



Transport of a pulse:
Flowthrough: t1 = turnover time = $\frac{\text{Surface film volume}}{\text{Water influx/year}}$

(Use average value of advective water flux)

Key Uncertain Parameters

Total system hydrology:
- Average percolation flux
- Variance across the repository
- Saturated hydraulic conductivity of rock matrix

Waste package hydrology:
- Fraction of local advective flux getting into waste package
- Fraction of fuel surface wetted

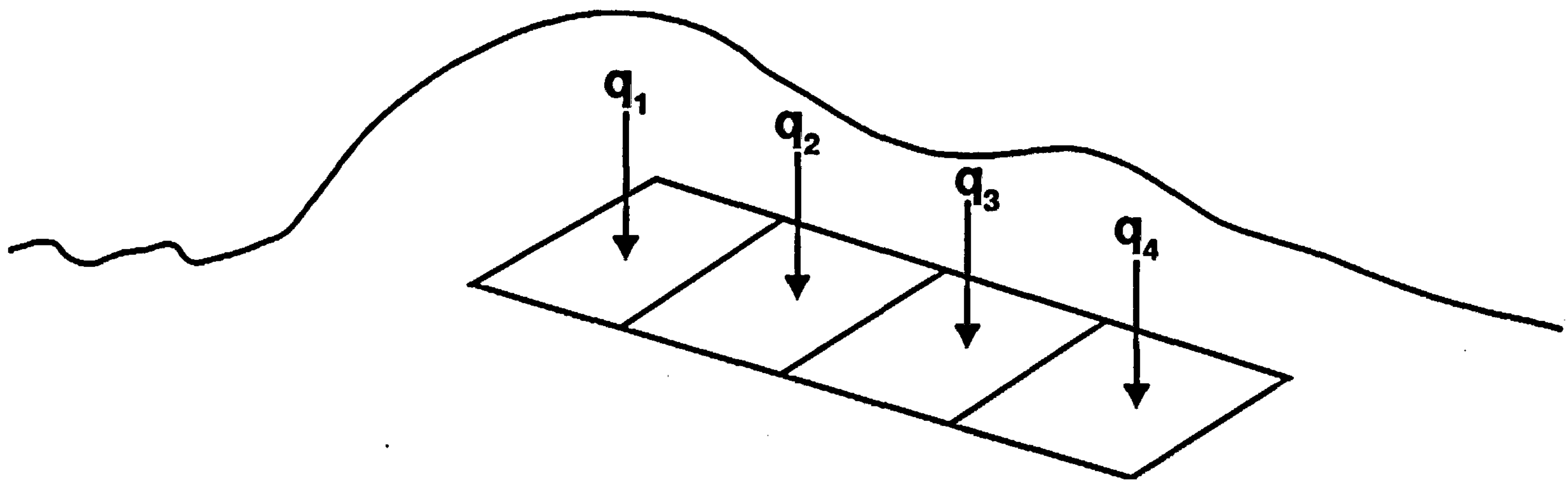
Rock mechanics:
- Fraction of boreholes with rubble
- Fraction of spent fuel exposed to diffusion

Diffusion hydrology and geochemistry:
- Effective diffusion coefficients
- Retardation factors

Geochemistry/waste-form interaction
- Fuel matrix alteration rate
- Element solubilities

Containers:
- Container failure rate

Area-Averaged Water Flux Affects Both Source Term and Far-Field Transport -- Correlations



- A trend in average water flux will introduce a correlation of source term strength and transport speed, and a de-facto correlation of these with transport path length to the water table
- Geochemical trends would probably also yield correlated changes in processes, but this was not explicitly modeled

Impacts of Hydrological Spatial Variability While Assuming a Matrix Flow Model

Assumptions:

- Lognormal distribution in space for the water flux
- Local excess flux goes into seepage flux
- Random spatial distribution of rubble occurrence

Results:

- Even a few % of waste packages with seepage flux will contribute most of the source term
- Hydrology-induced correlations among:
  - Container breach
  - Radionuclide release rate
  - Groundwater travel time to the water table

Impacts of Hydrological Spatial Variability, While Assuming a Fracture-Flow Model

Assumptions:

- A set of flows distributed in space and in amplitude; non-flowing zones have moist rock
- Random spatial distribution of rubble occurrence

Results are qualitatively similar to the matrix-dominated case