ATTACHMENT 3

NRC Staff - State of Nevada Meeting on NRC's Total-system Performance Assessment (TPA) Code

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Welcome and Introductions

- Welcome to State of Nevada (NV)
- Introductions of NV and NRC Participants
- Goals and Purposes of Meeting
- Opening Remarks
  - NRC
  - NV

NRC's Role

- Protect Public Health and Safety
- Independent Regulator of DOE
- NRC's TPA Code is a review tool developed to assist NRC staff in pre-licensing activities and reviewing a potential DOE license application

Role of NRC's TPA Code

- Independent review capability
  - Enhance understanding and evaluation of DOE's models, assumptions, and data
  - Flexibility to evaluate the completeness of DOE modeling approaches

- DOE has responsibility to demonstrate compliance with NRC's regulatory requirements

United States Nuclear Regulatory Commission

Overview of NRC's Total-System Performance Assessment (TPA) Code

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Presented to: Representatives of the State of Nevada
June 17, 2003

Presentation Overview

- TPA Code Overview
  - Execution, code requirements, etc.
- Summary of TPA Parameters, Assumptions, and Component Models
  - Nominal Scenario
  - Disruptive Scenarios
- Conclusions

TPA Code Overview

TPA: A Review Tool

- TPA is an **independent** tool used to support review of both pre-licensing activities and a potential license application.

- TPA uses available **data** to construct approaches based on first principles.

- TPA uses approaches that allow for **computational efficiency** where warranted.

- TPA uses approaches that allow for **flexibility** in the independent evaluation that would support the review of a license application for the proposed repository.

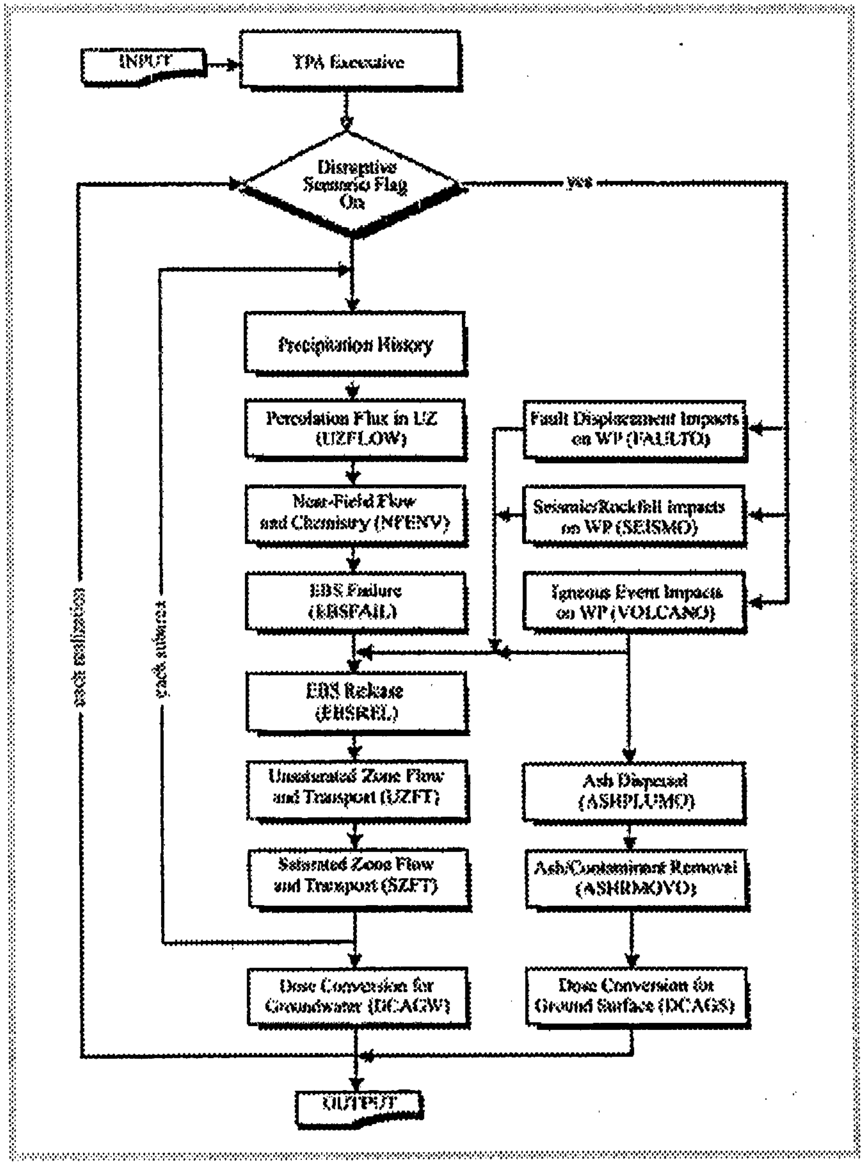
TPA Approach

- TPA conducts probabilistic dose calculations for specified time periods.
- Scenario classes include:
  - A nominal case including climate changes and seismic activity,
  - A disruptive case involving faulting*, and
  - A disruptive case involving igneous activity*.

* Assessment of risk from disruptive events must consider likelihood of occurrence of events

TPA Architecture

- TPA consists of:
  - Executive module that serves as the program driver.
  - An input module for reading the input file.
  - A set of consequence modules for:
    - The engineered components
    - The natural components
    - Disruptive scenarios
    - Receptor doses



TPA Execution

- TPA developed primarily for Unix platform
  - Code designed to be as portable as possible
  - TPA Version 4.1j code has been ported to Windows NT platform
  - Major compatibility issues not expected to exist
  - Written in FORTRAN
  - Compiled with Lahey FORTRAN 90 Version 4.5
- System Requirements
  - Windows NT v4
  - 128 MB RAM
  - 20 GB Disk Space
- Execution time
  - Example: 250 realizations for 10,000 years on a PC with a 2.4GHz processor and 1.6 GB of RAM took roughly 90 minutes

TPA Execution

- For each simulation,
  - EXEC first calls READER to read input data and check for errors
  - EXEC then checks for scenario class to be simulated and determines ordered sequence of module executions required

- For each realization,
  - EXEC calls SAMPLER to generate random vectors, with each vector consisting of a collection of the random independent parameters
  - EXEC invokes INVENT to determine initial radionuclide inventories and thermal loading

- For each subarea,
  - EXEC executes the consequence modules needed for a particular scenario

TPA Input Parameters and Sources

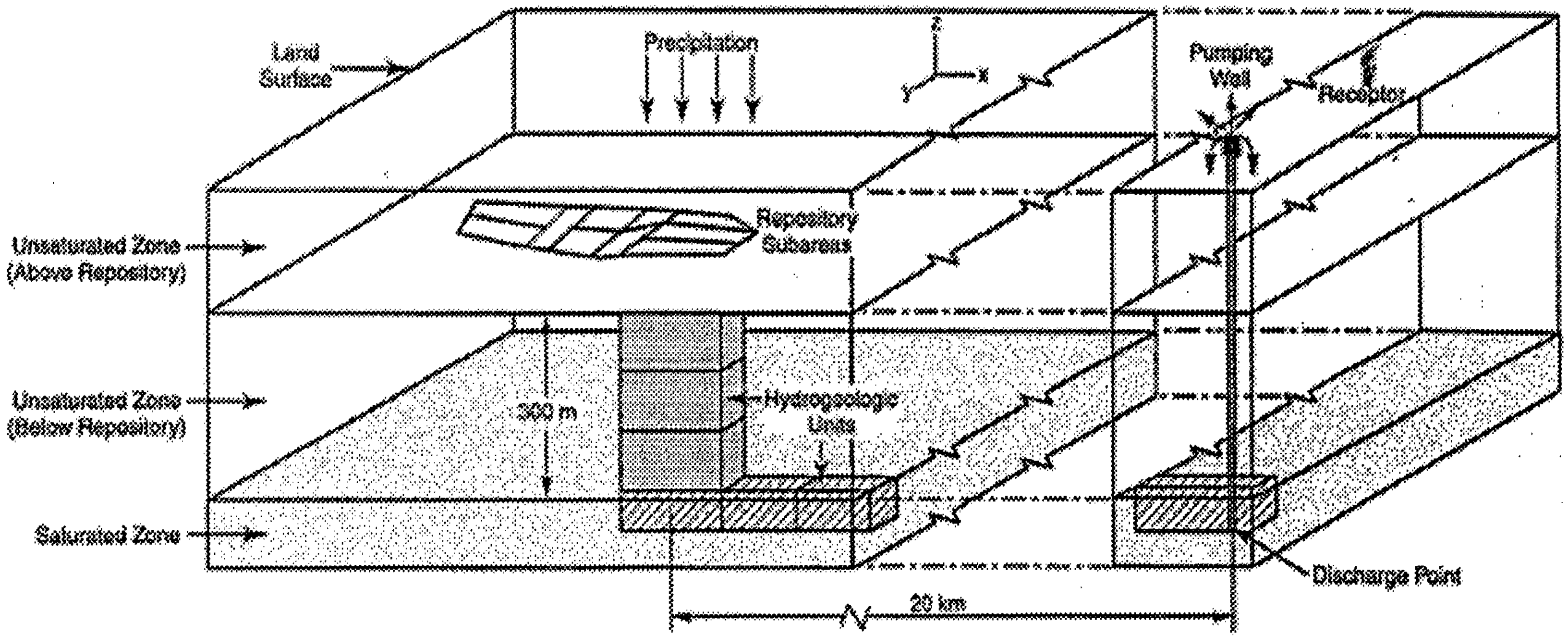
- APPENDIX A of the TPA User's Guide provides a reference data set.
- APPENDIX B of the TPA User's Guide provides auxiliary data files used during execution of the code.
- The main input file is ***tpa.inp***.
- Reference data set parameter values or distributions do not constitute regulatory acceptability.
- Input values can be assigned a diverse range of probability distribution types (e.g., twelve different types) and can be correlated.
- Latin Hypercube Sampling (LHS) used to sample the probability distributions.

TPA Outputs

- Many different types of output are produced during a code run:
  - Intermediate outputs (Appendix E, TPA User's Guide)
  - Sampled parameter values (*samplpar.res*)
  - Dose vs. time data for each realization
- Post processing of code output necessary:
  - TPA code produces consequences for disruptive events
  - Separate calculation needed to account for likelihood and develop risk
  - Total System Performance Assessment and Integration Issue Resolution Status Report Rev. 3 (September 2000) describes the procedure to calculate the risk from disruptive events

Summary of TPA Parameters, Assumptions, and Component Models

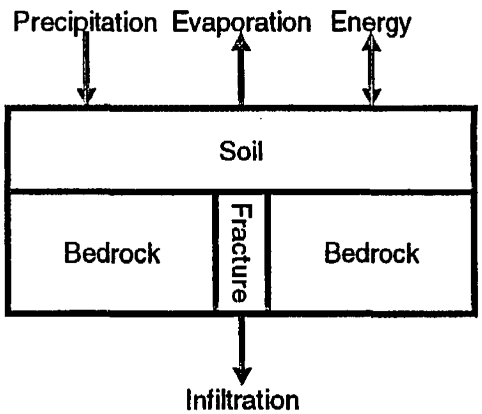
Repository Conceptualization

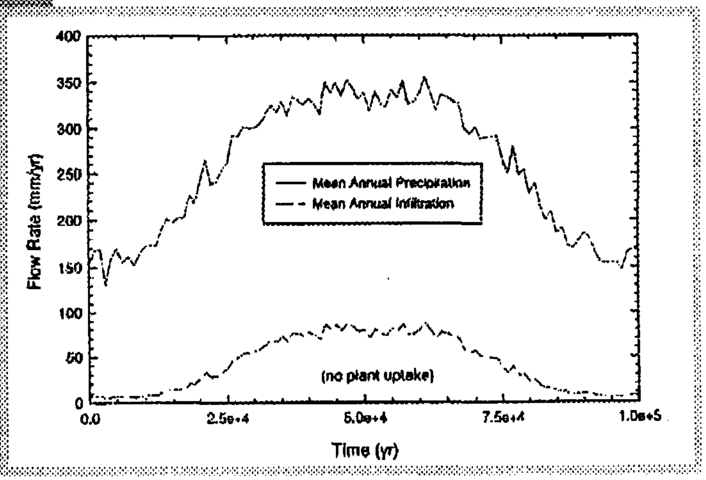


Water Movement Through the Repository

- Temperature and precipitation vary with glacial cycles.
- Process-level modeling estimates the shallow infiltration flux.
- Deep percolation flux equal to the shallow infiltration flux.
- Rate of water seeping into drifts can be modified by coupled processes such as vaporization, condensation, and refluxing.
- Other processes can influence quantity of water reaching the waste.

Shallow Infiltration

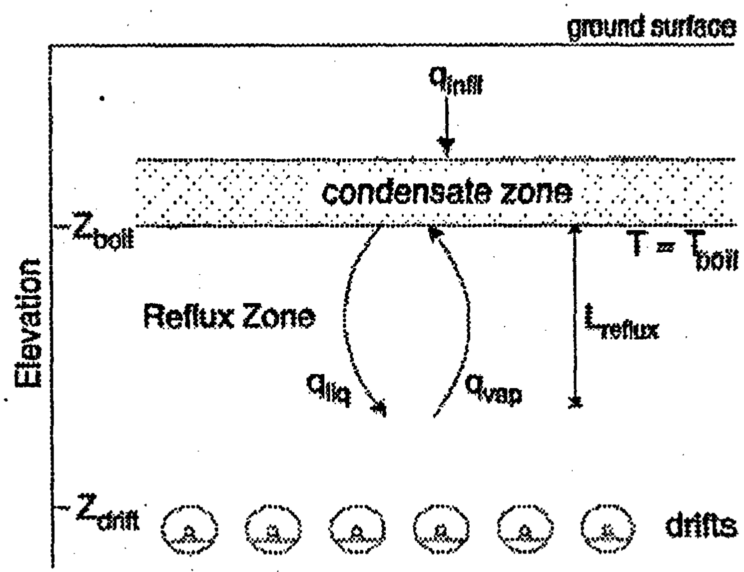




Variation of infiltration with climate change.

- Evidence suggests precipitation may have been 1.5-2.5 times larger than current climate conditions, while temperature may have been cooler by 5-10 ^{O}C at last full glacial maximum.
- Net infiltration for the modern climate is based on 1-D simulation results using a 15-year record of hourly meteorological data from Desert Rock, Nevada.
- Process-level modeling, which incorporates climate, soil depth, and bedrock permeability, estimates the shallow infiltration flux for bare-soil conditions.

Groundwater Reflux



Conceptualization of drift-scale thermal hydrologic model.

- Process-level thermohydrologic modeling calculates the thickness of the dry out zone above the repository for TPA.
- Theory suggests water flowing down a fracture could penetrate a distance below the boiling isotherm before completely vaporizing.
- Water reaches the drift when the penetration distance exceeds the thickness of the dry out zone.
- TPA also incorporates two additional alternative conceptualizations to model groundwater reflux.

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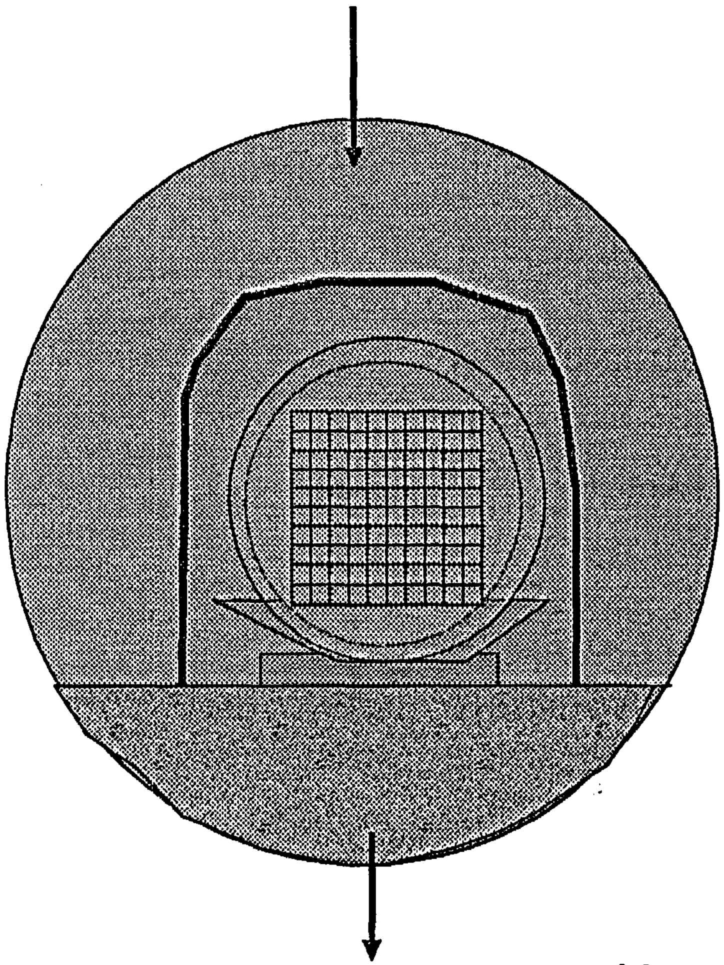
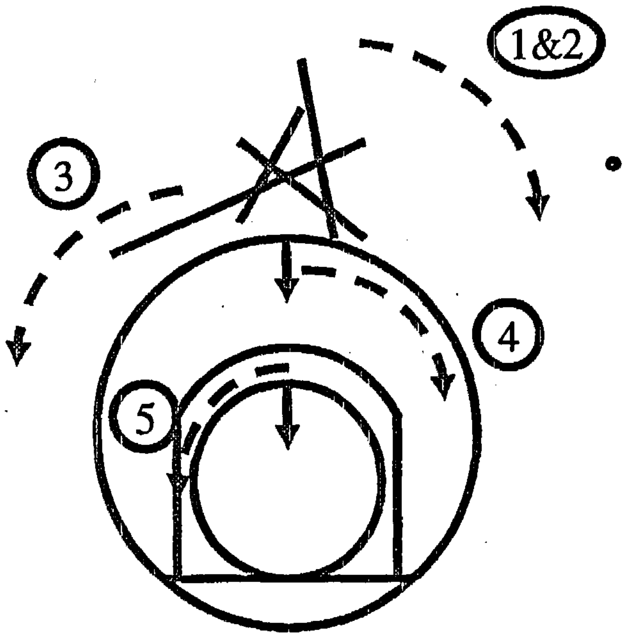
Water entering drift



- Seepage and water contacting waste
- Drip shield corrosion
- Waste Package corrosion
- Spent fuel degradation
- Cladding failure
- Radionuclide Release

Water and radionuclides exiting the drift

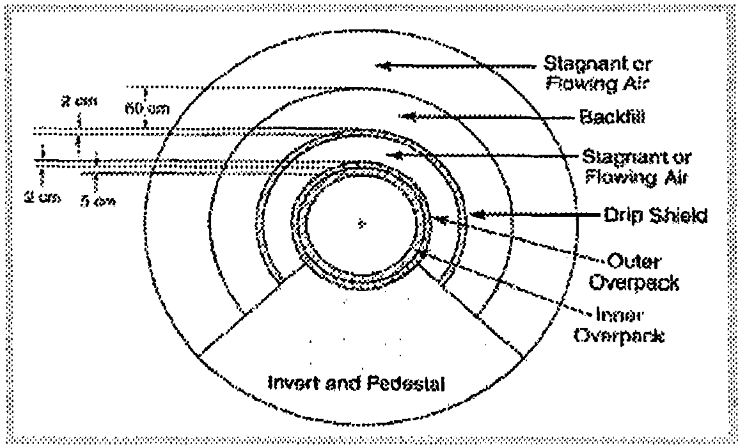
Flow Convergence/Divergence



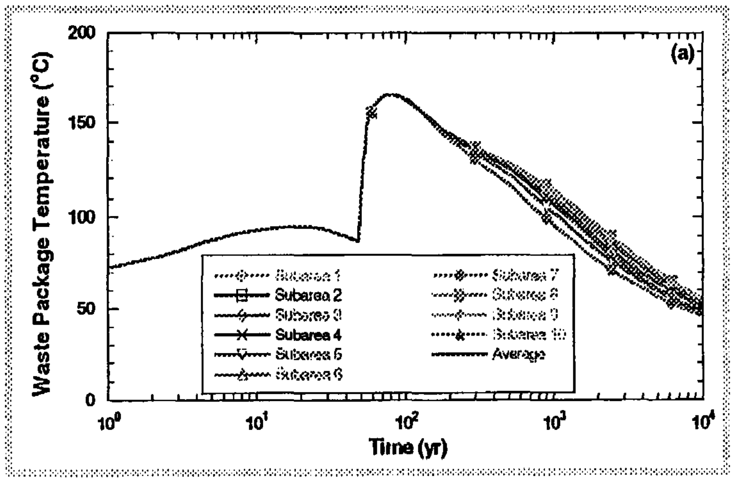
- TPA utilizes a simple and efficient approach to modify the percolation flux that reaches the waste package.
- Factors account for*:
  1. Fraction of waste packages dripped on,
  2. Focusing/divergence of deep percolation toward/away from drifts,
  3. Divergence due to capillary forces in unsaturated rocks,
  4. Film flow down the surface of the drift walls,
  5. Drips missing holes in the waste package, and the presence of corrosion products in the holes.

* Correlations can be important

Thermal Modeling



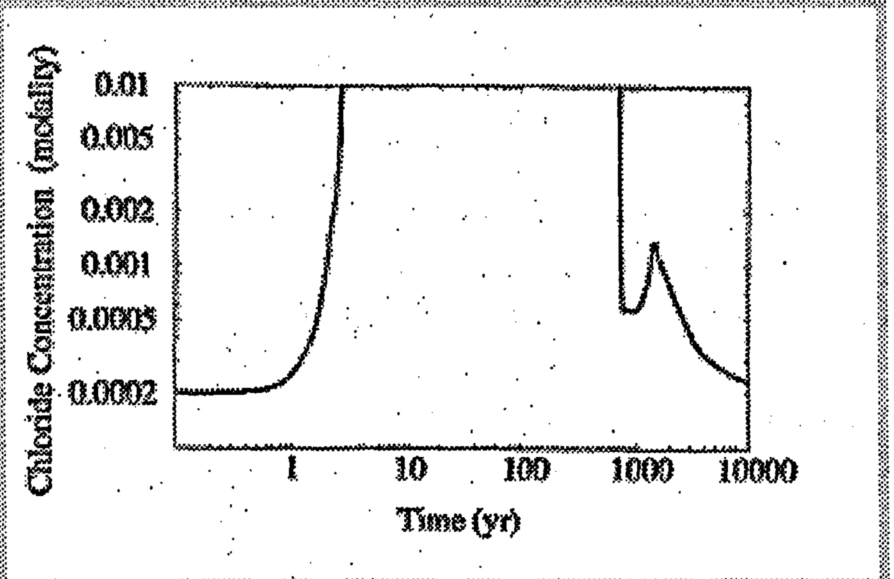
Idealization for thermal calculations.



Waste package surface temperatures.

- TPA calculates the temperature of the drift wall using a mountain-scale analytic conduction-only model.
- TPA calculates the waste package surface temperature and maximum temperature of the spent fuel using analytical approximations of multimodal heat transfer.
- TPA calculates RH as a function of drift wall and waste package surface temperatures and moisture present at closure.
- TPA can incorporate an alternative thermal model.

Near-Field Chemical Environment



Chloride concentration at the drift wall.

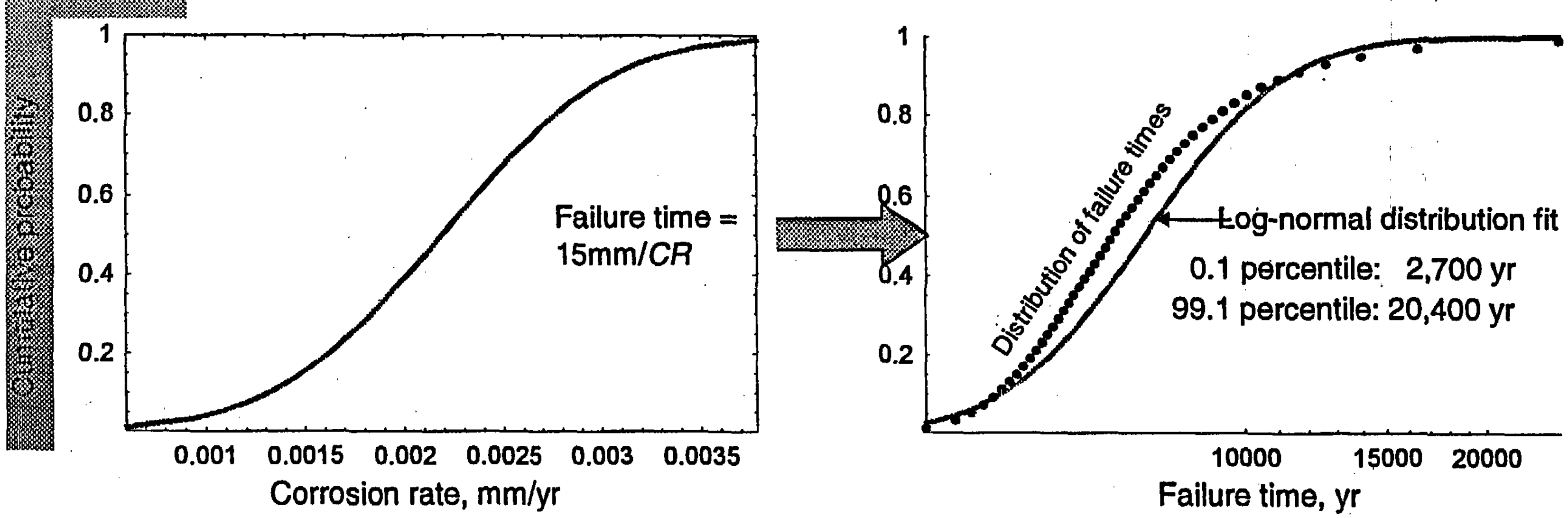
- Currently, process-level modeling simulates the change in chloride concentration due to evaporation.
- TPA adjusts the chloride concentration to account for uncertainties and limitations of the modeling to represent the chemistry on the waste package surface.
- TPA fixes pH at 9 based on process-modeling.

Engineered Barrier Degradation

- Process-level modeling estimates the time of drip shield failure.
- Temperature and the chemical environment on the waste package influence the mode and rate of corrosion.
- TPA calculates the waste package surface temperatures based on thermal output and the repository horizon temperature.
- Process-level modeling estimates the chemical environment on the surface of the waste package.
- Fabrication defects or emplacement damage may result in releases from a small number of waste packages prior to repository closure.

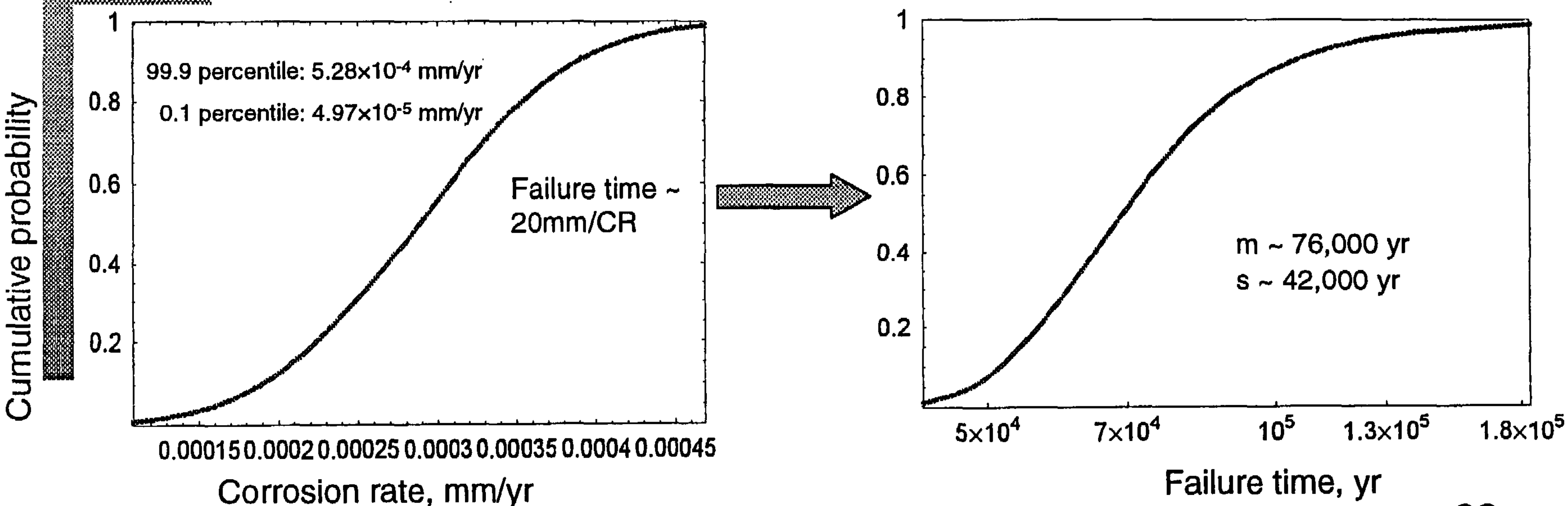
Drip Shield Corrosion

- Ti Grade 7 current densities in the range 10^{-8} to 5×10^{-7} A/cm^2 (pH range 2.1 to 10.7, [Cl] range 0.1 to 1M, 95°C)
- Corrosion rates ranging from 8.7×10^{-5} to 4.3×10^{-3} mm/yr (assumed 0.1 and 99.9 percentiles of a normal distribution)
- Assumptions: general corrosion occurs from only one side of the drip shield and is the only degradation mechanism

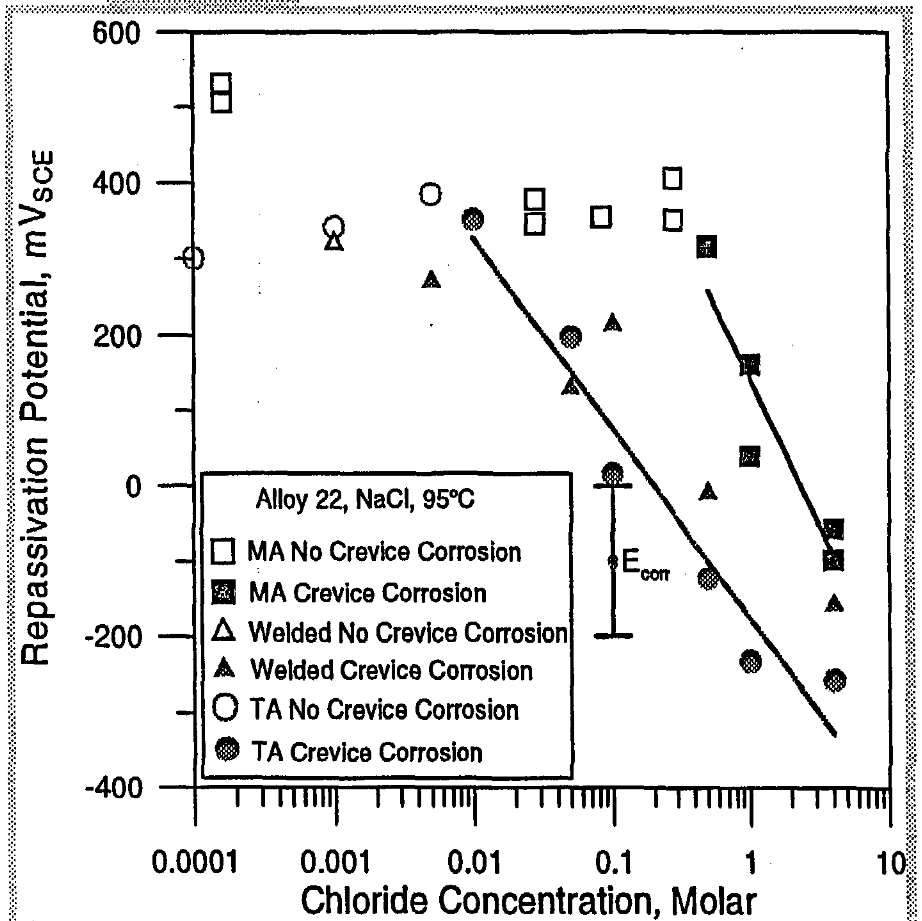


Waste Package – Uniform Corrosion

- Passive current densities in the range 5×10^{-9} A/cm^2 to 5.4×10^{-8} A/cm^2 (pH range 2.7 to 8, [Cl] range 0.028 to 4 M, 95°C)
- The corrosion rate in the code is computed using Faraday's law.
- Corrosion rates ranging from 4.97×10^{-5} to 5.28×10^{-4} mm/yr (assumed 0.1 and 99.9 percentiles of a normal distribution)
- Assumptions: failure defined to occur as complete penetration of the waste package wall thickness by the corrosion front



Waste package – localized corrosion



MA – Mill Annealed
TA – MA + Aged 5 minutes at 870 °C
Welded – MA + Welded

- Localized (crevice) corrosion occurs when the corrosion potential (E_{corr}) is higher than the crevice corrosion repassivation potential (E_{rcrev})

$$E_{rcrev} = E^o_{rcrev}(T) + B(T) \log[Cl^-]$$

where $E^o_{rcrev}(T)$ and $B(T)$ are linear functions of temperature

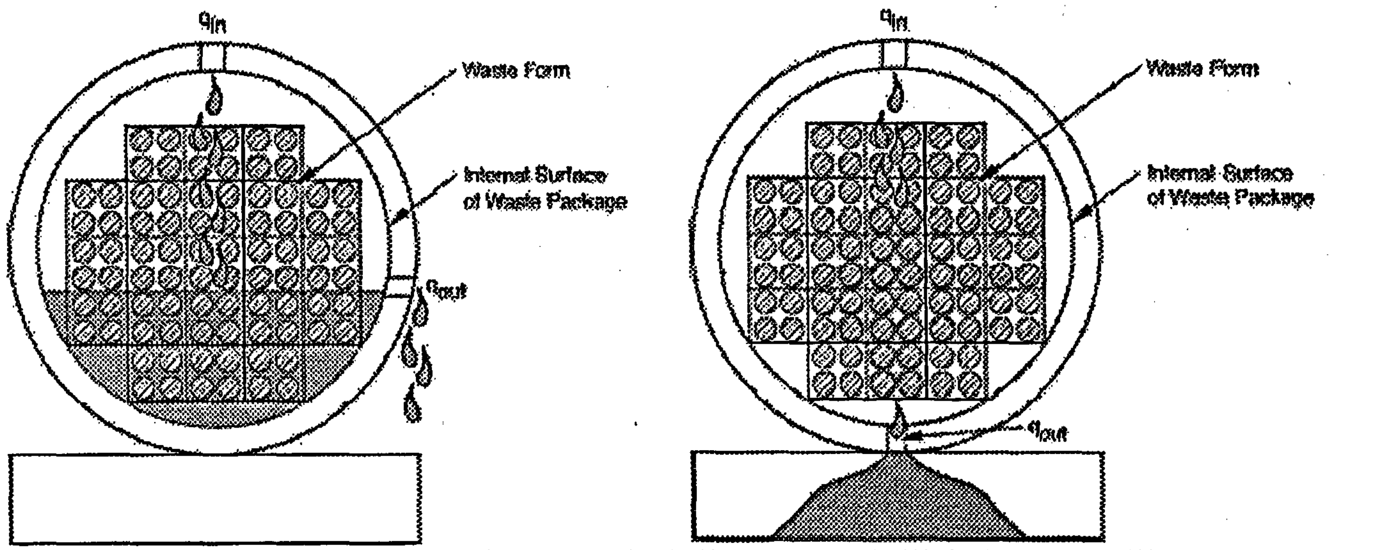
- As a result of welding and post-welding processes, E_{rcrev} may become lower than E_{corr}, facilitating the occurrence of localized corrosion
- These effects, as well as the inhibiting effect of NO_3^-, can be introduced in the code through changes in the E_{rcrev} expression

Waste Package – Stress Corrosion Cracking (SCC)

- For the conditions evaluated and types of tests performed, stress corrosion cracking has not been observed.

- Flexibility to analyze SCC is present in the code through the initial defects model.

Conceptual Models for Water Contact



- Bathtub and flow-through conceptual models for water contacting the waste.
- Bathtub modeled as a stirred-tank. Solubility limits are applied to both models.

Waste Form - Spent Nuclear Fuel (SNF)

- The NRC has 4 different models in TPA for SNF dissolution.
  - Models based on experimental data for different conditions (model 1 and model 2), natural analogs (model 3), and secondary mineral formation [schoepite] (model 4).
  - Base case is Model 2 (T=25 to 85 °C, J-13 and carbonate solutions)
  - Temperature dependence from spent fuel tests under immersion and flow through conditions at 25 and 85 °C (Wilson 1990; Gray et al. 1992)
  - Two models for SNF surface area: particle and grain.

$$r = r_o \exp[-E_a/RT]$$

E_a=activation energy [kJ/mol]
r_o=pre-exponential coefficient [mg/m^2-d]
R=universal gas constant [kJ/mol-K]
T= WP temperature [K]

Waste Form – Cladding

- The failure mechanisms of cladding include (i) mechanical failure by external forces, (ii) localized corrosion, (iii) creep, (iv) hydrogen-induced failure, (v) splitting by matrix volume expansion, (vi) uniform corrosion, (vii) creep, and (viii) stress corrosion cracking.
- TPA4.1j has a factor (CladdingCorrectionFactor) to represent the fraction of the spent fuel surface area protected by cladding.
- CladdingCorrectionFactor is set by the code user for complete to no protection.
- Approach allows flexibility and ease of use.

Release and Transport Out of the Package

- Transport out of waste packages is by advection.
- Two models for aqueous release of radionuclides are available for selection by the user: bathtub and flow-through.
- Flow-through model is the same, but (1) doesn't allow buildup of fluid, and (2) the fraction of fuel wetted is independent of water level.
- Release is: $M_{out}[i]=Q \cdot C[i]$

  where Q is the water flow rate and C[i] is the concentration of radionuclide i in solution.
- Solubility limits abstraction is based on (i) the likely solid phase precipitated or co-precipitated and (ii) the chemistry of the fluid that reacts with the solid phase.

Release and Transport Out of the Package

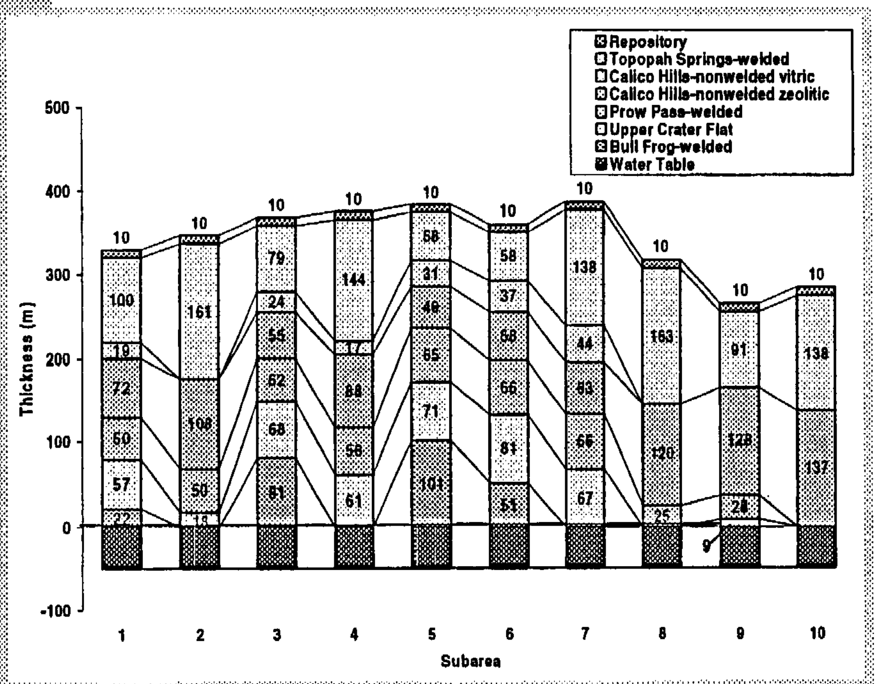
- For a number of radio-elements (C, Cs, Cl, I, Se, Tc) solubility limits are set to 1.0 M because no solubility-limiting solids are estimated to form.

- The range and probability distributions of solubility limits for many other elements in TPA are based on an elicitation of experts conducted by DOE in 1993 (Wilson et al., 1994, CRWMS M&O, 1998).

- The assumptions behind the expert panel's distributions are:
  - the UZ water composition is bounded by that of J-13 well water and well UE-25p#1.
  - the solubility limits are determined by far-field groundwater environment.
  - the environment is oxidizing.

- TPA has a model for transport through the invert (simple advection/retardation/diffusion model) and a factor to bypass transport through the invert for high flow rates.

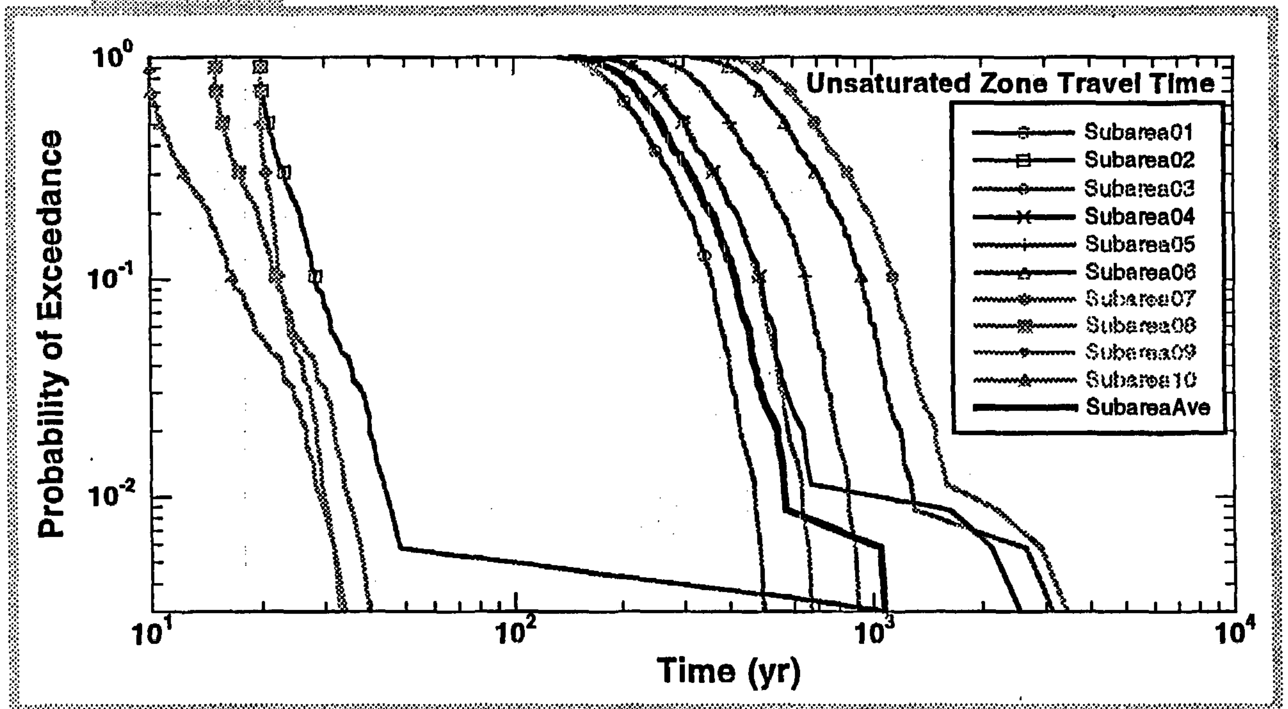
Unsaturated Radionuclide Transport



Unsaturated Zone Hydrostratigraphic Thicknesses.

- TPA utilizes a simple 1-D vertical flow field through hydrostratigraphic layers whose thicknesses were derived from the Geologic Framework Model 3.1.
- UZ flow occurs in fractures when the percolation flux exceeds the matrix hydraulic conductivity for a given tuff layer.
- TPA does not include diffusion of radionuclides from fast flowing fractures into near-stagnant matrix pores.
- TPA models retardation in the rock matrix.

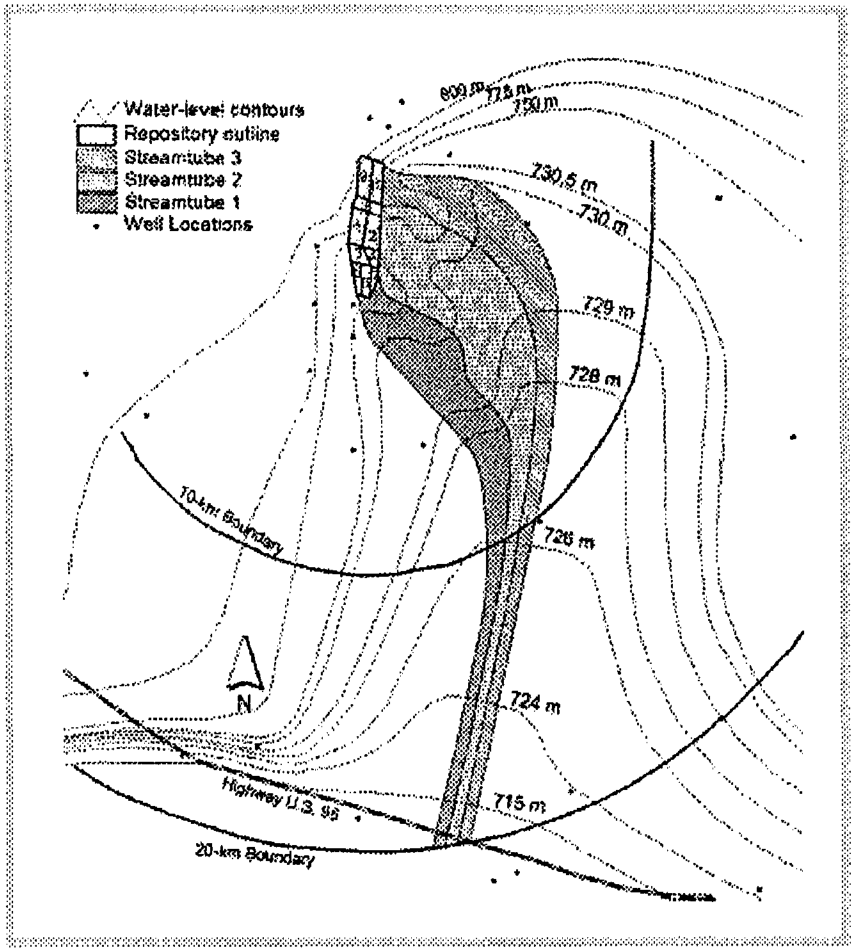
Unsaturated Radionuclide Transport



Unretarded unsaturated zone travel time.

- Assumes no retardation in fractures.
- May bypass UZ for efficiency (based on travel time)

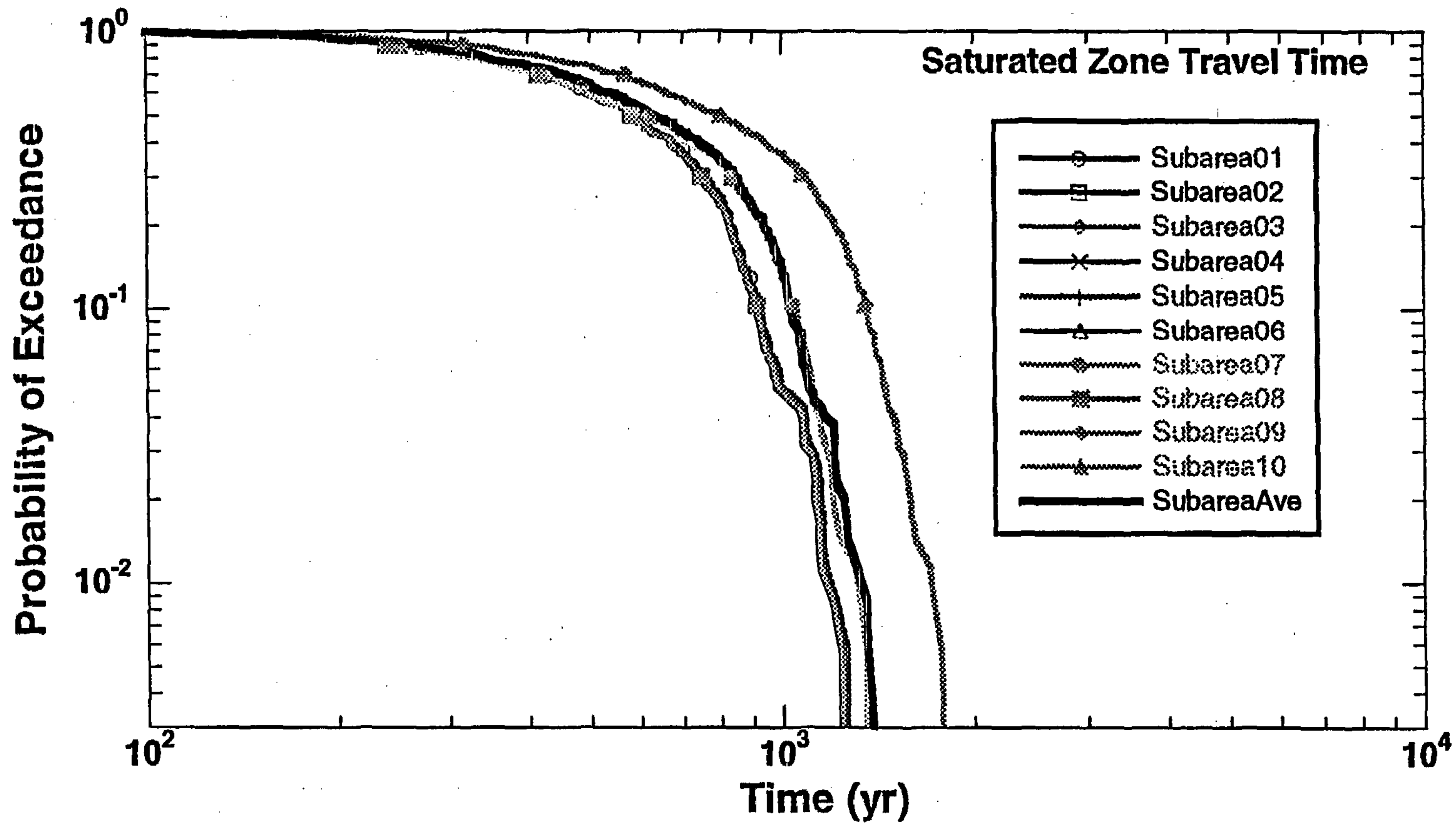
Saturated Radionuclide Transport



Saturated zone streamtubes.

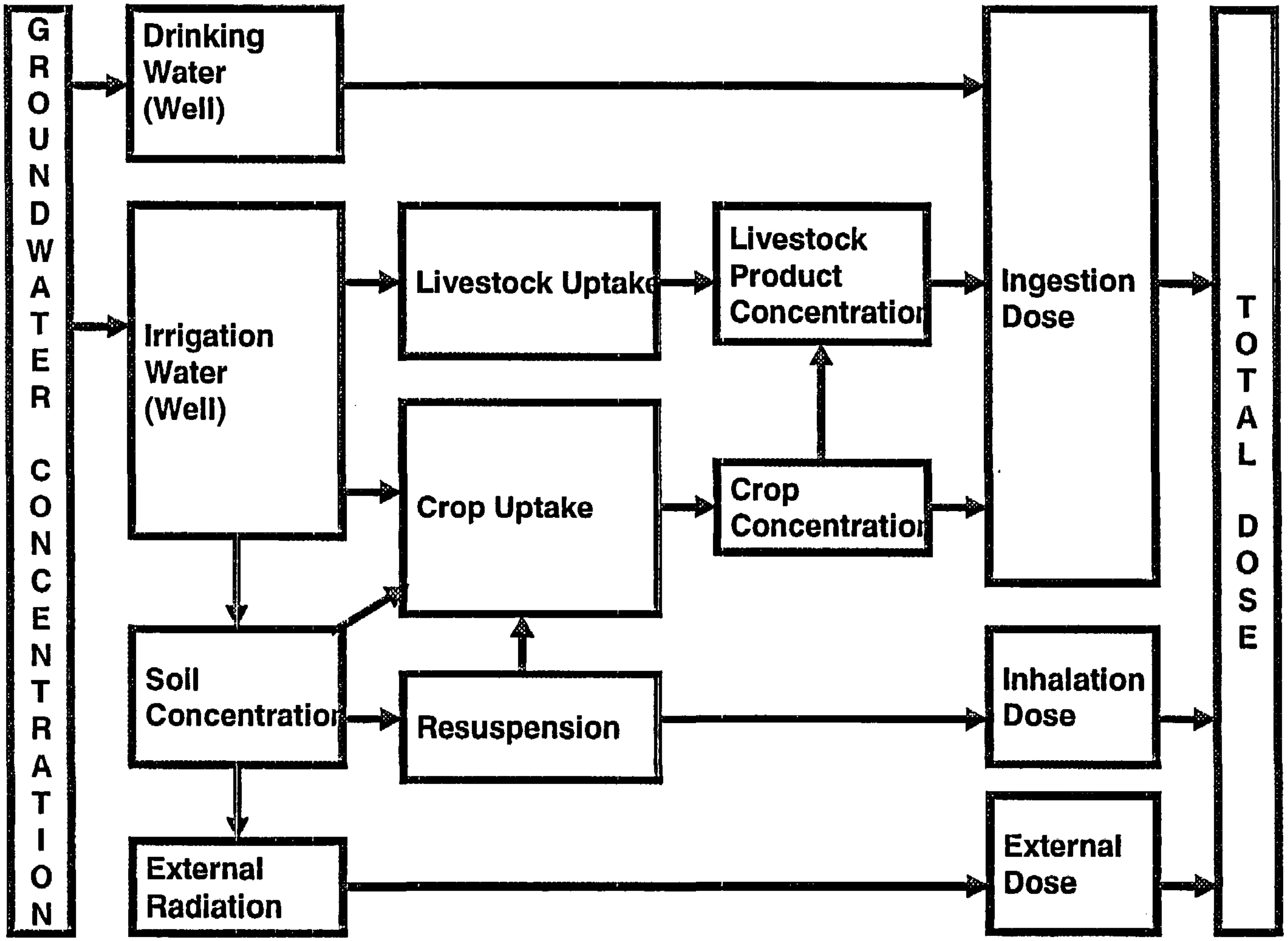
- TPA models 3 streamtubes based on a 2-D horizontal flow-net interpretation of hydraulic gradients in the uppermost aquifer.
- Water level data from area wells provides basis for hydraulic gradient and transmissivity.
- TPA samples tuff-alluvium interface.
- TPA models sorption in alluvial aquifer and tuff matrix.
- Radionuclides can diffuse from fractures into matrix in the tuff aquifer.

Saturated Radionuclide Transport



Unretarded saturated zone travel time.

Consideration of Exposure Pathways



Disruptive Events

Igneous Activity

- TPA calculates **consequences** of extrusive and intrusive releases of radionuclides
    - separate calculations are necessary to develop the **risk**

- Extrusive Release – radionuclides entrained in magma are transported by volcanic ash

- Intrusive Release – waste packages are damaged by magma in drifts and radionuclides can be transported by water contacting the waste

Extrusive Release

- Number of Waste Packages Impacted
  - two models (geometric or "user" specified)
  - entire inventory is assumed to be entrained in the magma
- Transport of Radionuclides by Ash
  - Suzuki model describes the areal density of accumulated ash
  - incorporation ratio used to distribute radionuclides in ash
- Evolution of Ash Deposit
  - accounts for leaching, erosion, and radioactive decay
- Dose Calculation
  - greatest contribution due to inhalation
  - mass loading variable over time (highest the first year)

Chapters 14, 15, 16, & 17 – VOLCANO, ASHPUMO, ASHRMOVO, and DCAGS

Intrusive Release

- Number of Waste Packages Impacted
  - Geometric model (based on dike length and location)
  - "user" specified distribution
- Waste Package Damage
  - all waste packages contacted by magma are assumed to be damaged
  - fraction of waste form contacted by water (set by user)
- Radionuclide Release and Transport via Ground Water
  - seepage and unsaturated flow are assumed to be unaffected by igneous event

Faulting

- Number of Waste Packages Impacted
  - Geometric model (based on fault length, width, and location)

- Waste Package Damage
  - waste packages assumed damaged when minimum fault displacement exceeded
  - fraction of waste form contacted by water (set by user)

- Radionuclide Release and Transport via Ground Water
  - seepage and unsaturated flow are assumed to be unaffected by fault movement
  - can assume a separate “fault zone” sub-area for transport

Seismic Activity

- Dynamic effects of rockfall cause mechanical damage to the waste package
  - rock conditions (size of rock blocks that fall)
  - distance that rock falls
  - mechanical strength of waste package (impact stress induces plastic strain exceeding 2 percent)

- Waste Package Damage
  - waste package damage assessed over 4 different time periods
  - fraction of waste form contacted by water (set by user)

- Radionuclide Release and Transport via Ground Water
  - seepage and unsaturated flow are assumed to be unaffected by seismicity

TPA Review and Verification

- The TPA code has been developed, tested, and documented under a quality assurance program
- Peer review of TPA 3.2
  - Areas evaluated
  - Key recommendations
  - Staff follow-up
- Past analyses with and verification of the TPA code

Conclusions

- TPA code is used as a **review** tool. Licensing decisions and conclusions will be based on DOE's TSPA.

- Understanding and explanation of PA results is an essential aspect to developing confidence in PA models.

- TPA provides a **flexible** framework to independently evaluate the performance of a potential Yucca Mountain repository system.

Select References

S. Mohanty, T.J. McCartin, and D.W. Esh. "Total-System Performance Assessment Code (TPA), Version 4.0 Code: Module Descriptions & User's Guide." San Antonio, Texas, USA: Center for Nuclear Waste Regulatory Analyses. 2002.

Issue Resolution Status Report Key Technical Issue: Total System Performance Assessment and Integration, Revision 3. 9/28/2000. (ML003754539)

S. Mohanty, R. Codell, R.W. Rice, J. Weldy, Y. Lu, R.M. Byrne, T.J. McCartin, M.S. Jarzemba, and G.W. Wittmeyer. "A System-Level Repository Sensitivity Analyses Using TPA Version 3.2 Code." CNWRA 99-002. San Antonio, Texas, USA: Center for Nuclear Waste Regulatory Analyses. 1999. (ML012990108 & ML012990118)

S. Mohanty, R. Codell, J. Menchaca, R. Janetzke, M. Smith, P. LaPlante, M. Rahimi, and A. Lozano. "System-level performance assessment of the proposed repository at Yucca Mountain using the TPA version 4.1 code", CNWRA 2002-5, revision 1. (Expected to be publicly available 2003)

J. Weldy and J. Peckenpaugh, "Response to the External Peer Review of the Total-system Performance Assessment Version 3.2 Code." San Antonio, Texas, USA: Center for Nuclear Waste Regulatory Analyses. revised 2003.

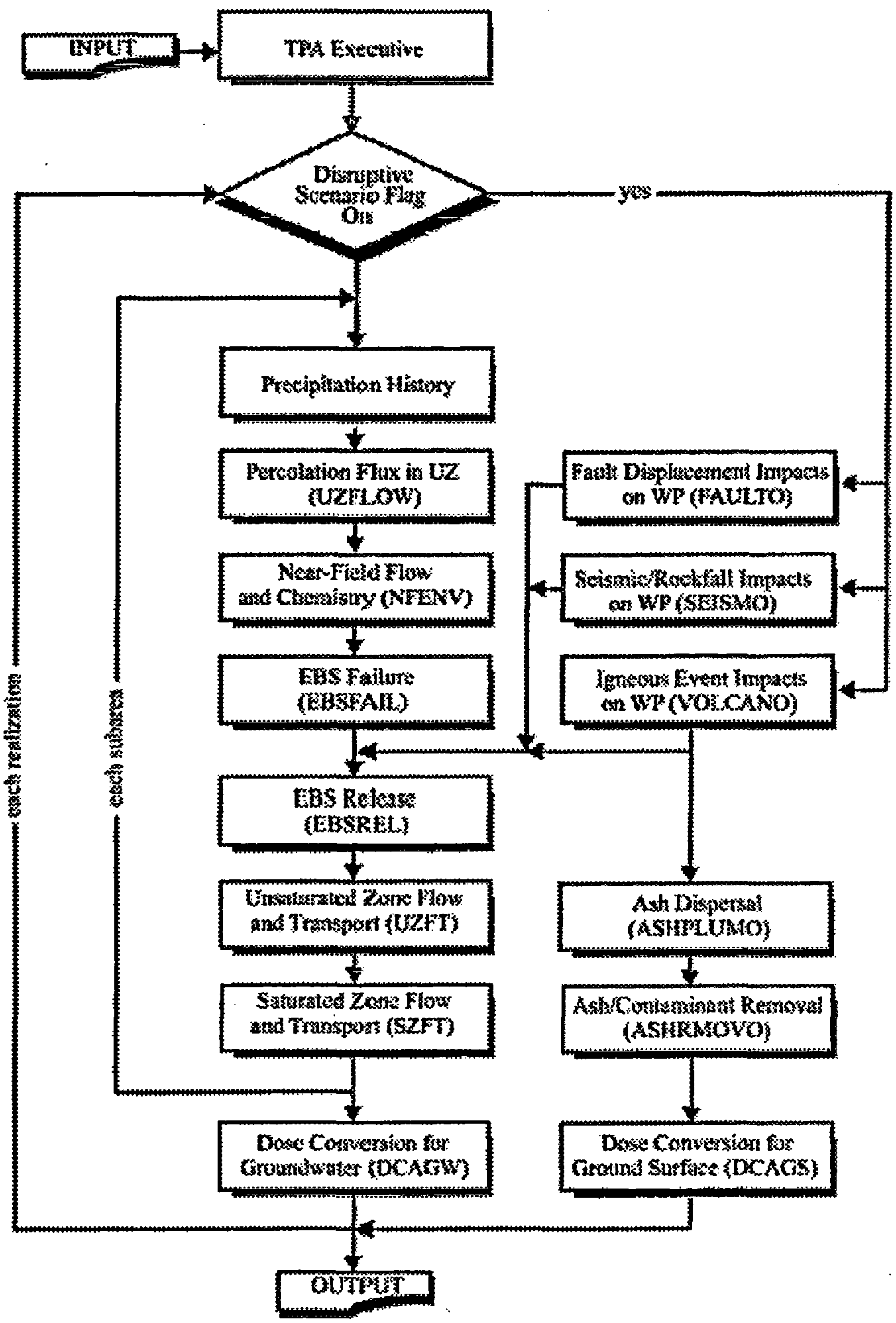


Figure of TPA Code Architecture