U.S. Department of Energy
Office of Civilian Radioactive Waste Management

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# Implementation of Localized Corrosion in the Performance Assessment Model for Yucca Mountain

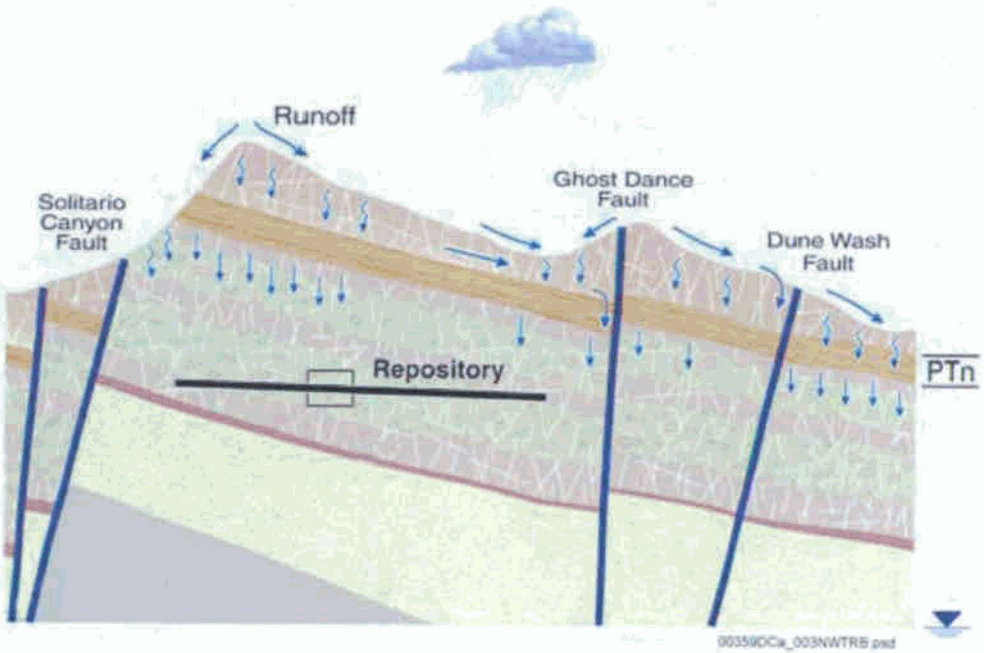
## 2006 International High Level Radioactive Waste Management Conference


Presented by:
**Vivek Jain[1], S. David Sevougian[2] , Patrick D. Mattie[2], Kevin G. Mon[3] and Robert J MacKinnon[2]**
**[1]Bechtel SAIC LLC**
**[2]Sandia National Laboratories**
**[3]Areva NP, INC**

# Presentation Outline

- Description of proposed Yucca Mountain repository
- Description of localized corrosion process
- Localized corrosion initiation model
- Abstraction and modeling methodology
  - Coupling of models
  - Quantification of uncertainty and variability
  - Issues of scaling and variability
  - Implementation in Yucca Mountain Performance Assessment model
- Summary

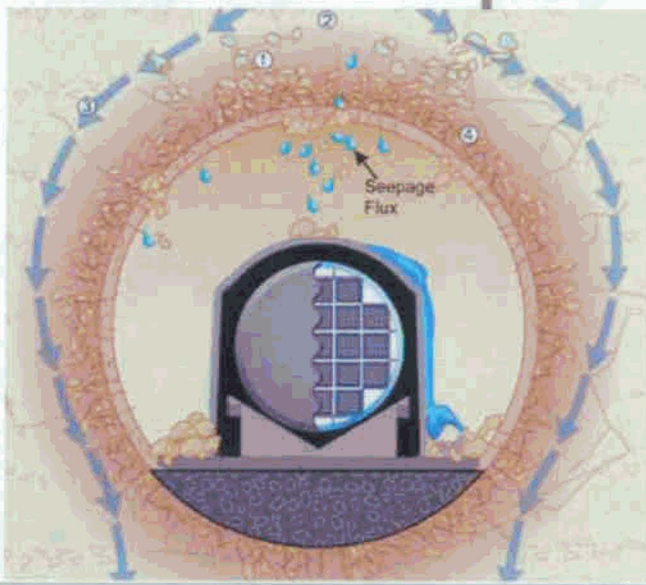
# Natural System of Yucca Mountain

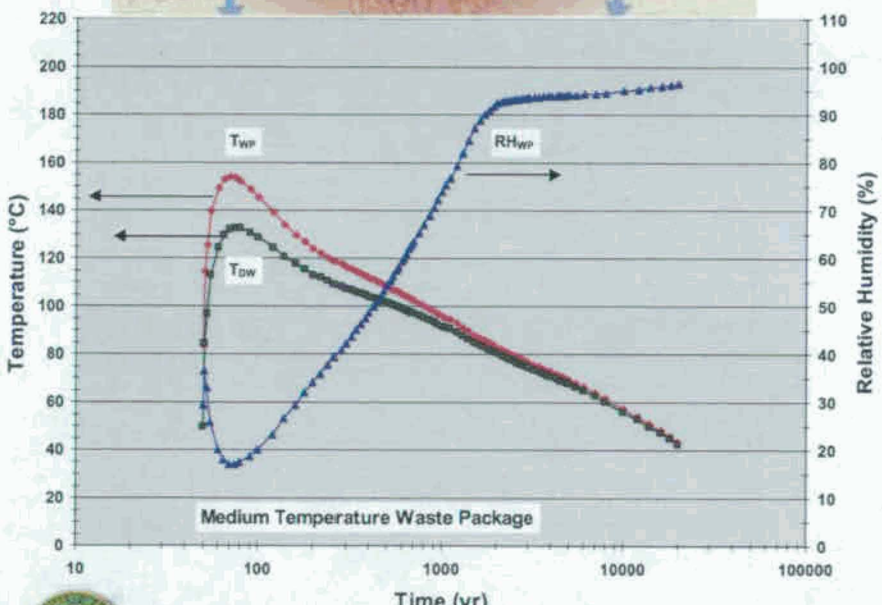



## Important Factors

- Waste packages are isolated beneath ~300 meters of rock and ~300 meters above the water table.
- Repository in Unsaturated Zone
  - Fractured porous rock
  - Pores partially filled with water
- Atmospheric pressure
- Relative humidity ranges from low to high; limited dripping
- Ambient waters are dilute and near neutral pH
- Highly concentrated waters can form under proposed repository conditions

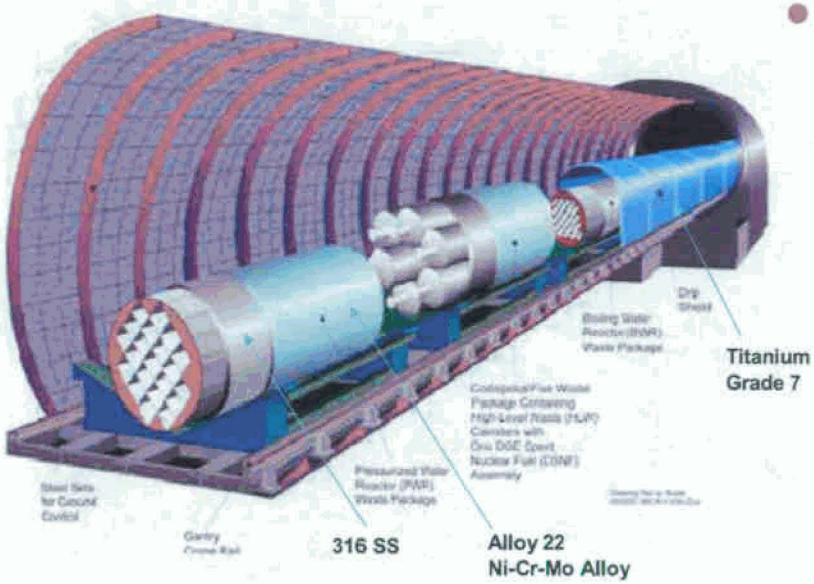
# Attributes of Proposed Yucca Mountain Repository



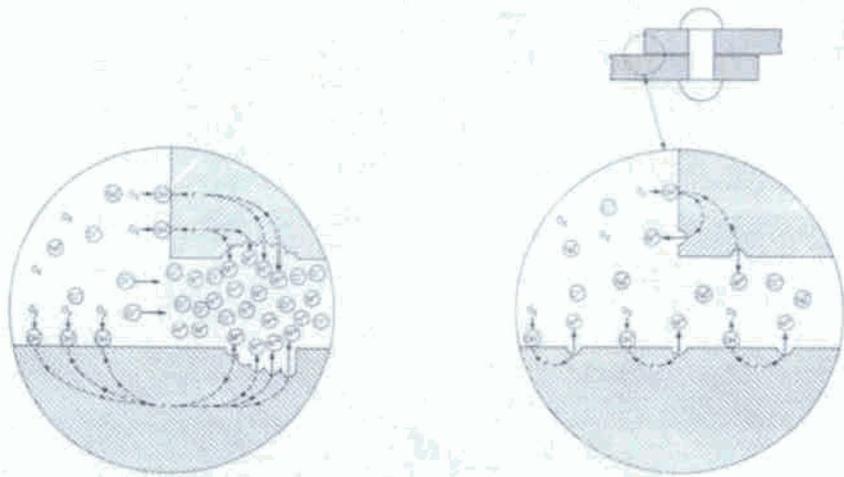

- One long, slow cycle of heating to modest temperature and cooling to ambient
- Waste packages on support pallets
- No rapid thermal expansion and contraction
  - Low heat fluxes
  - Slow heating and cooling
  - Modest thermal gradients
- Heat and radiation from waste decrease with time
  - Radiation effects at waste package surface negligible after a few hundred years
  - Packages cool to ambient over several thousands of years
- Limited amount of water moving through the rock
- Limited salts and minerals carried into drifts by incoming water

# Localized Corrosion of Alloy 22



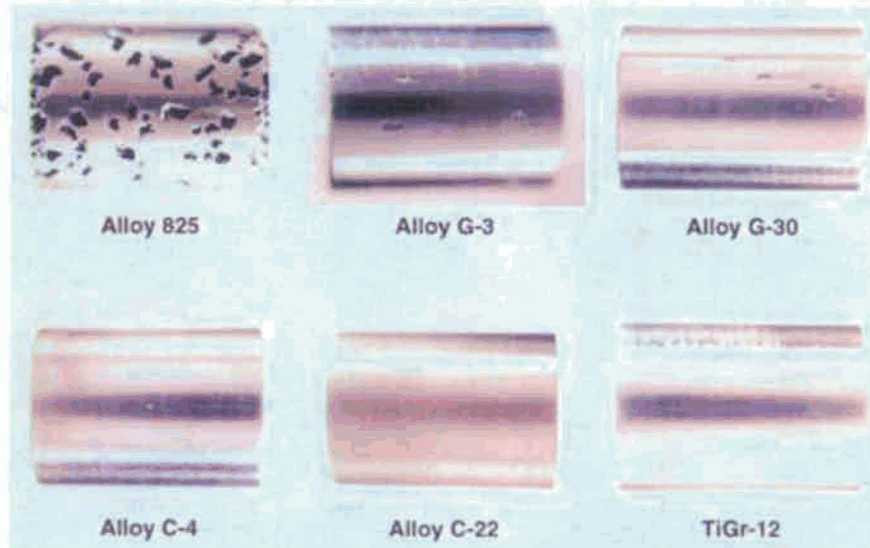

- Outer shell of the waste package is of Alloy 22
- Alloy 22 belongs to a family of Ni-Cr-Mo alloys
  - Earlier alloys include C-276 and C-4 and later alloys include: Inconel 686, Alloy 59, Hastelloy C-2000 and MAT-21
  - Alloy 22 (N06022) is a solid solution of Ni, Cr, Mo and W as the main alloying elements
- Cr-Mo-W in Alloy 22 act synergistically to provide resistance to localized corrosion such as crevice and pitting corrosion

# Description of Corrosion Process



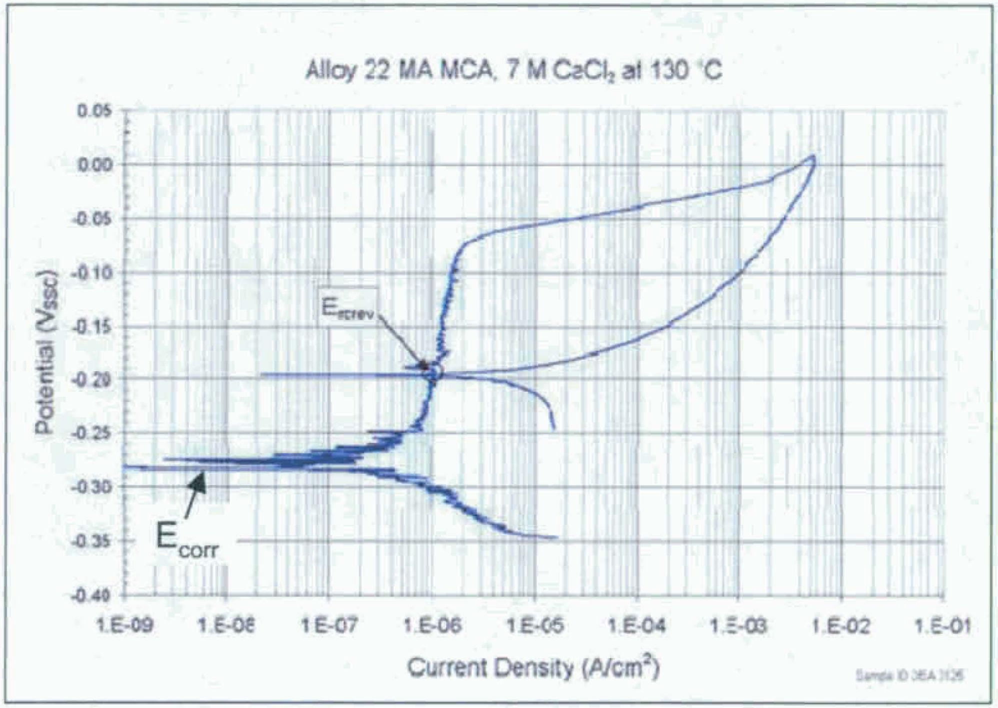
(After Fontana *Corrosion Engineering)*

## Pitting Susceptibility of Candidate WP Outer Shell Materials




**Surfaces after potentiodynamic polarization in acidified (pH 2.7) 10%NaCl at 90 C**

# Localized Corrosion Initiation Model




Mill-Annealed Alloy 22 Tested in 7 *M* $CaCl_2$ Solution at 130°C

- **Localized corrosion initiation model uses empirical regression equations for corrosion potential ($E_{corr}$) and crevice repassivation potential ($E_{rcev}$), from cyclic potentiodynamic polarization (CPP) tests**
- **Localized corrosion initiates when:** $\Delta E = (E_{rcrev} - E_{corr}) \leq 0$

# Variables for Crevice Corrosion

- Crevice corrosion depends on
  - Chloride concentration ($Cl^-$)
  - Nitrate concentration ($NO_3^-$)
  - Temperature (T)
  - Potential (E)
  - Acidity (pH)
  - Crevice geometry (tightness)
- The higher the $Cl^-$, T, E; the lower the pH and $NO_3^-$; and the tighter the crevice geometry $\Rightarrow$ the lower the resistance of alloys to crevice corrosion

# Localized Corrosion Initiation Model (cont.)

- **Localized corrosion initiates when:** $\Delta E = (E_{rcrev} - E_{corr}) \leq 0$
- **Crevice repassivation potential ($E_{rcrev}$) is given as**

$$E_{rcrev} = E^{o}_{rcrev} + \Delta E^{NO_3^-}_{rcrev}$$

**where $E^{o}_{rcrev}$ is the crevice repassivation potential in the absence of inhibitive nitrate-ions, and $\Delta E^{NO_3^-}_{rcrev}$ is the crevice repassivation potential change resulting from the inhibiting effect of nitrate in solution.**

- **Crevice repassivation potential:**

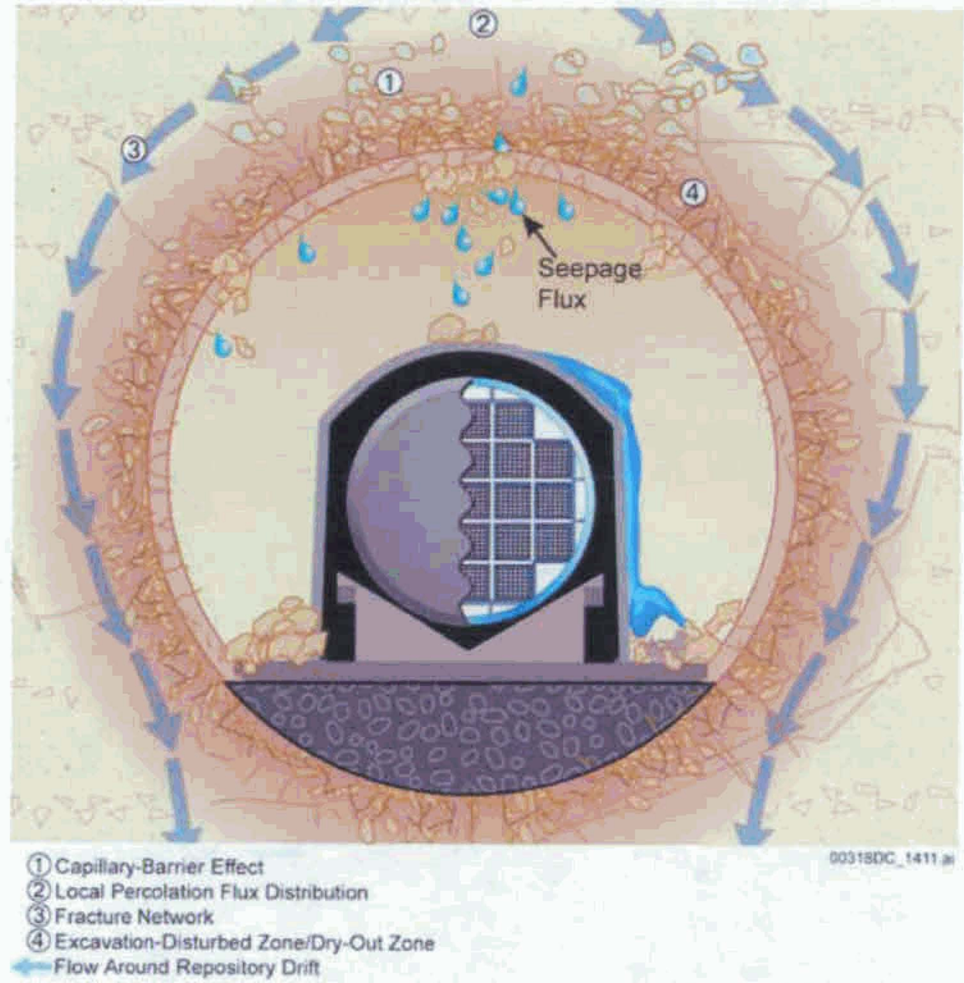
$$E_{rcrev} = E_{rcrev}(T, pH, Cl^-, NO_3^-, \frac{NO_3^-}{Cl^-})$$

- **Long-term corrosion potential:**

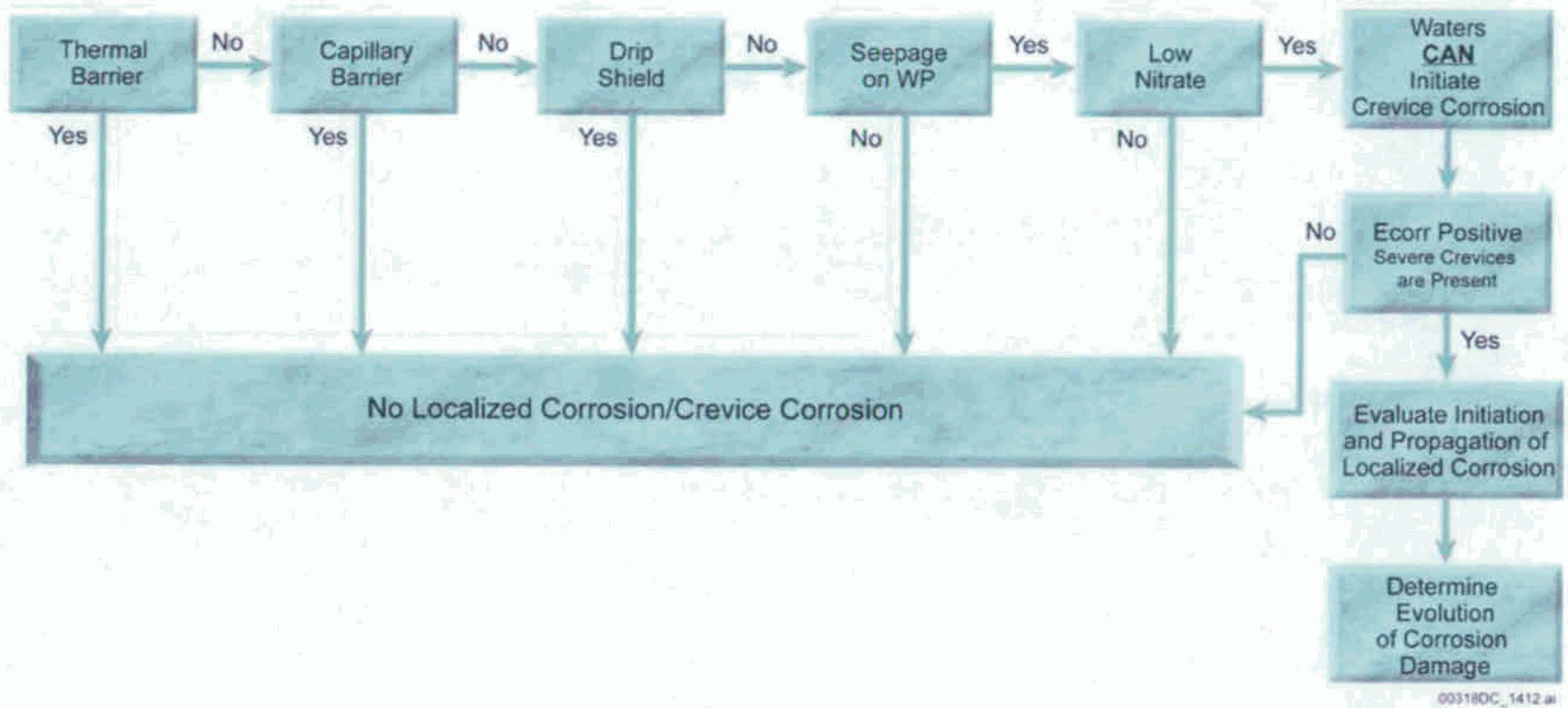
$$E_{corr} = E_{corr}(T, pH, Cl^-, \frac{NO_3^-}{Cl^-})$$

# Factors that Protect Against Corrosion

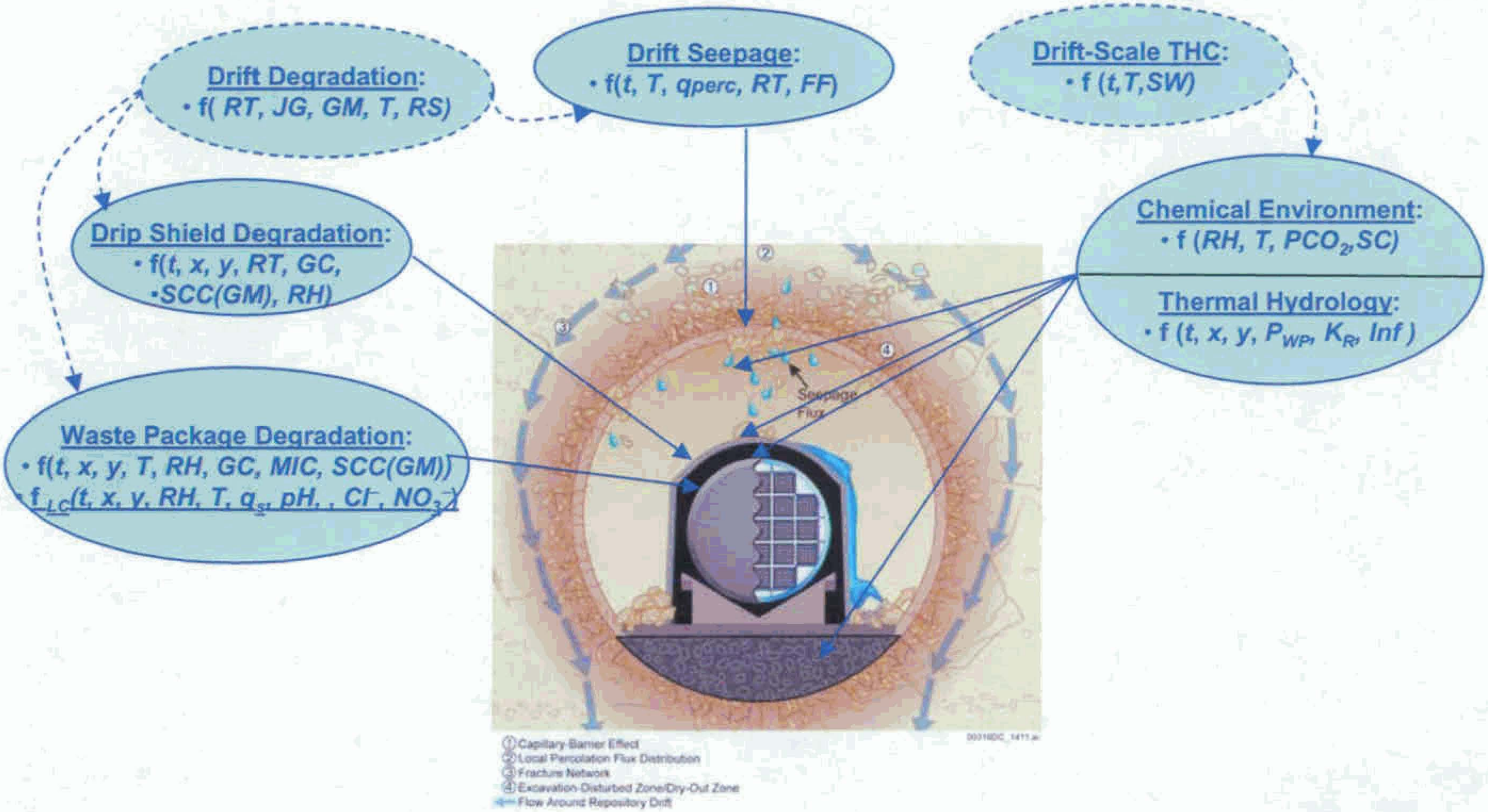
- Thermal barrier
  - Drift wall above boiling temperature
  - No drips onto waste package
- Capillary barrier
  - Water retained by unsaturated rock
  - No drips onto waste package
- Drip shield
  - No drips onto waste package
- Highly corrosion-resistant Alloy 22
  - No significant corrosion in absence of dripping
  - No corrosion in a wide range of waters resulting from dripping



# Localized Corrosion Decision Tree



# EBS Models/Processes Needed for Localized Corrosion



# Coupling of EBS Localized Corrosion Initiation Model with Environmental Input Models & Abstractions

**Drift Seepage Abstraction**
$Q_{seep}$ vs. time

**EBS TH Environment Submodel**
$T_{WP}$ vs. time
$RH_{WP}$ vs. time
$\Delta T_{WP}$ vs. time
$\Delta RH_{WP}$ vs. time
$T_{DW}$ vs. time
Lithophysal Flag
$Q_{PERC}$ vs. time

**EBS Chemistry Abstraction**
TSPA Look-up Tables
Crown Seepage
pH, $Cl^-$, $NO_3^-$ as f($RH, T, P_{CO_2}$, time)
RH threshold f($T, P_{CO_2}$, time)

**LC Initiation Abstraction**

**Localized Corrosion Initiation Analysis $\Delta E$ vs. time**

Example of coupling for one waste package at one repository location, including uncertainty

Number of Realizations →

Time ↓

| Time (years) | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 |
| 100 | 0 | 0 | 1 | 0 |
| 200 | 1 | 0 | 1 | 1 |
| 500 | 0 | 0 | 0 | 1 |
| 750 | 0 | 0 | 0 | 1 |
| 1000 | 0 | 1 | 0 | 1 |
| 1250 | 1 | 1 | 0 | 1 |

No Localized Corrosion = 0 (in table)

Localized Corrosion Initiated = 1 (in table)

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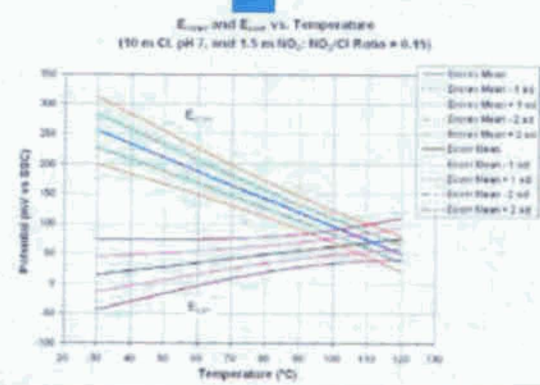
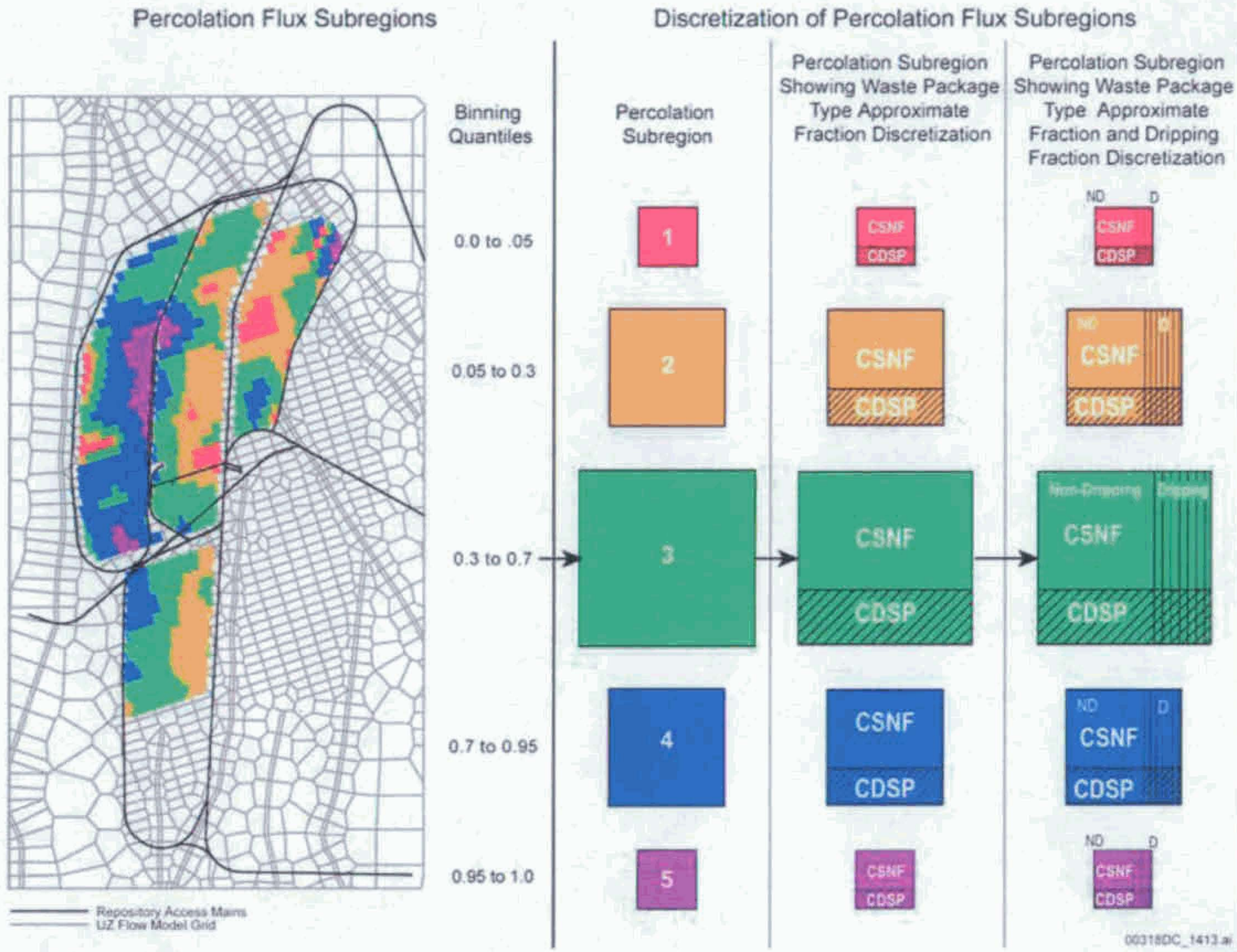


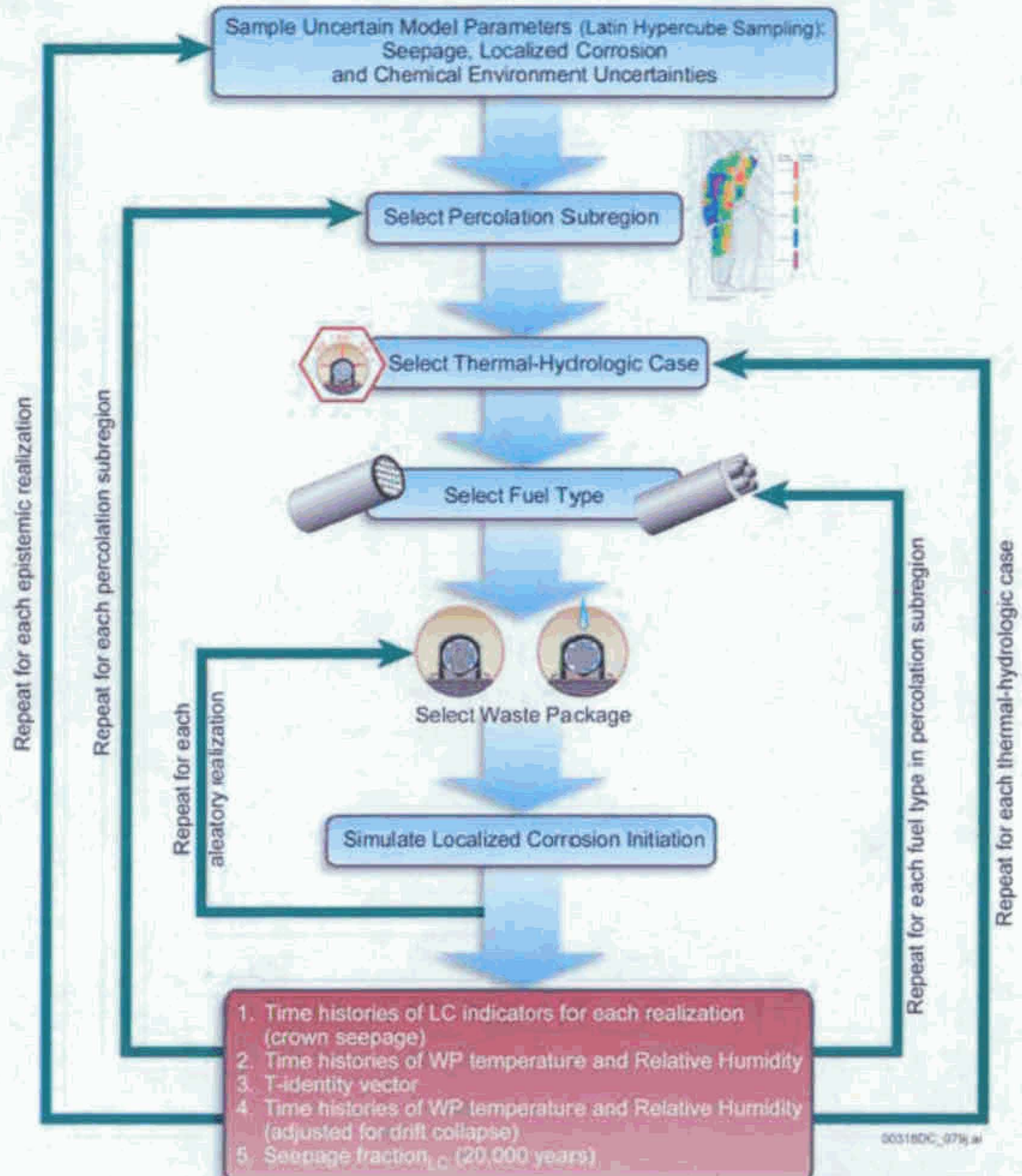
# Treatment of Variability and Uncertainty



# Treatment of Variability and Uncertainty (Cont.)

- Aleatory uncertainty (including spatial variability) refers to inherent unpredictability and randomness in the repository system and is considered to be irreducible.
- Epistemic uncertainty arises from a lack of knowledge about parameters and models, which can be reduced by additional testing and data collection.
- LC initiation analysis includes two computational loops:
  - outer epistemic uncertainty loop
    - sampling is performed on 24 uncertain epistemic parameter distributions (e.g. LC model coefficients, chemical parameters etc)
  - inner spatial variability loop
    - sampling is performed on 4 parameter distributions (e.g.: drift seepage parameters, temperature time histories etc)

# Implementation and Connection of Localized Corrosion Initiation Model, Uncertainties, and Variabilities in Yucca Mountain Performance Assessment



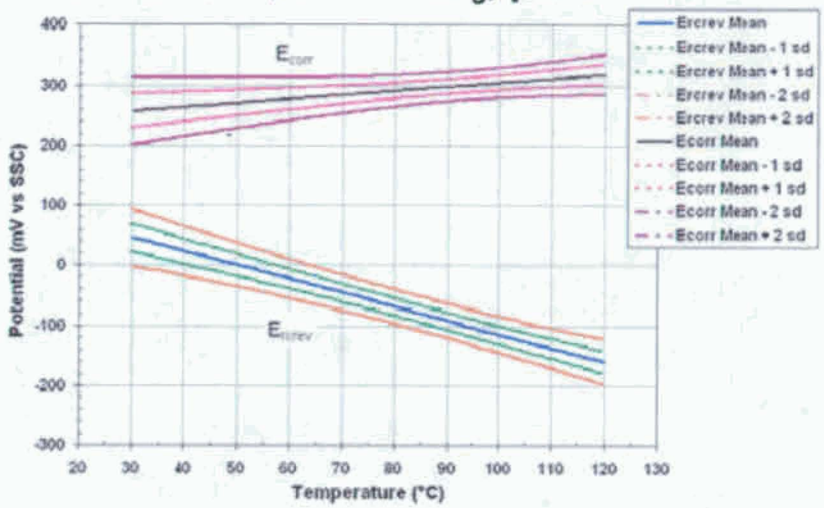

U = uncertainty

$V_R$ = variability (representative or upscaled)

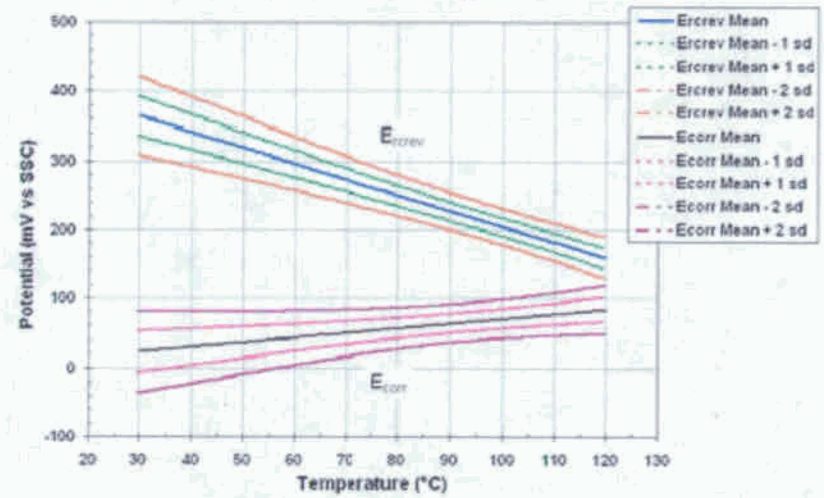
$V_D$ = variability (detailed or fine-scale)

# Example of LC Initiation Model Calculation

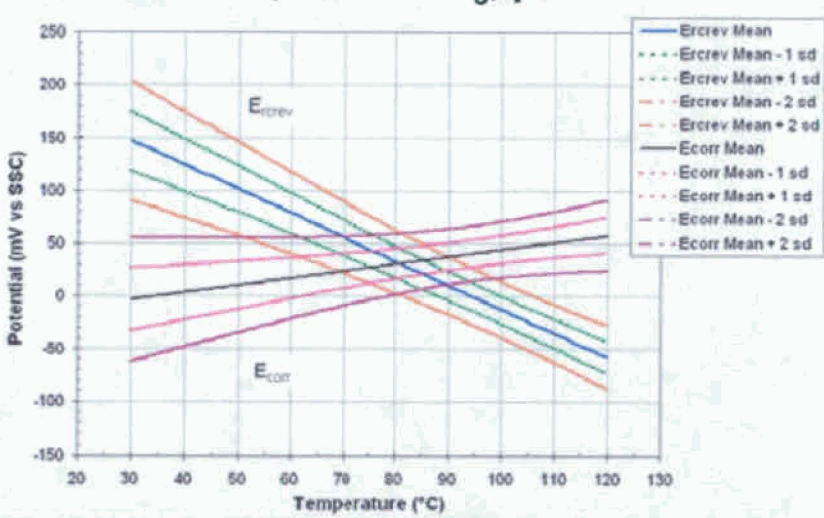
## 10 m Cl, 0.5 m $NO_3$, pH 3



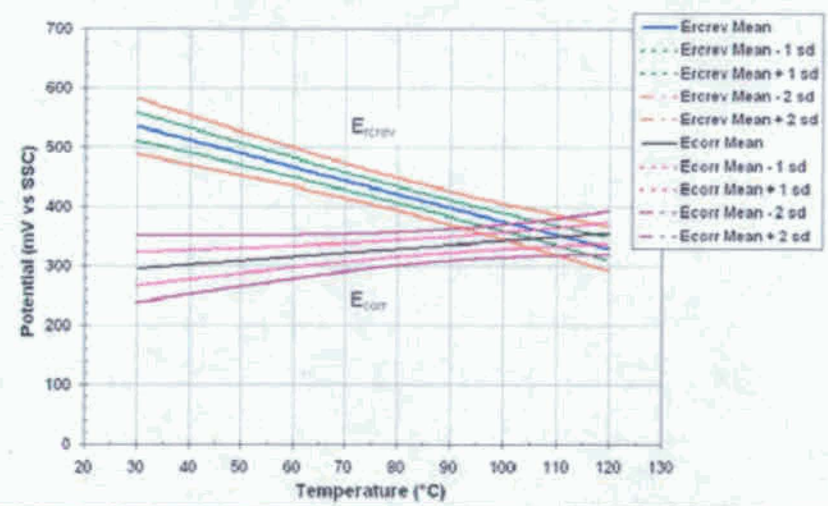

## 10 m Cl, 2.5 m $NO_3$, pH 7




## 10 m Cl, 0.5 m $NO_3$, pH 7




## 10 m Cl, 5.0 m $NO_3$, pH 3



# Summary

- Outer shell of waste package is made up of Alloy 22, which is highly resistant to corrosion
- Crevice corrosion can occur under extreme conditions
- Localized corrosion initiation model includes dependence on temperature, pH, chloride concentration, and nitrate concentration
- Localized corrosion model implementation incorporates a wide range of conditions on the waste package Alloy 22 outer shell :
  - Varying chemistry
  - Temperature
  - Spatial variability
  - Uncertainty in submodels

# Summary (cont.)

- Coupling of the LC submodel within the Yucca Mountain Performance Assessment model is complex because of the numerous processes involved
- By using various levels of discretization for uncertainty and variability as appropriate to the processes involved, the problem is implementable in a multi-realization, Monte Carlo performance assessment model.