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

NUCLEAR WASTE TECHNICAL REVIEW BOARD
EBS PANEL MEETING

SUBJECT: CORROSION MODELS IN PERFORMANCE ASSESSMENT

PRESENTER: DR. WILLIAM G. HALSEY

PRESENTER'S TITLE AND ORGANIZATION: TECHNICAL AREA LEADER, PERFORMANCE ASSESSMENT
LAWRENCE LIVERMORE NATIONAL LABORATORY
LIVERMORE, CA

PRESENTER'S TELEPHONE NUMBER: (510) 423-1133

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NUCLEAR WASTE TECHNICAL REVIEW BOARD
EBS PANEL MEETING

Corrosion Models in Performance Assessment

WILLIAM G. HALSEY
LLNL

Pleasanton, Ca.

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Outline

EBS Subsystem Performance Assessment
- Existing Models
- Use in TSPA

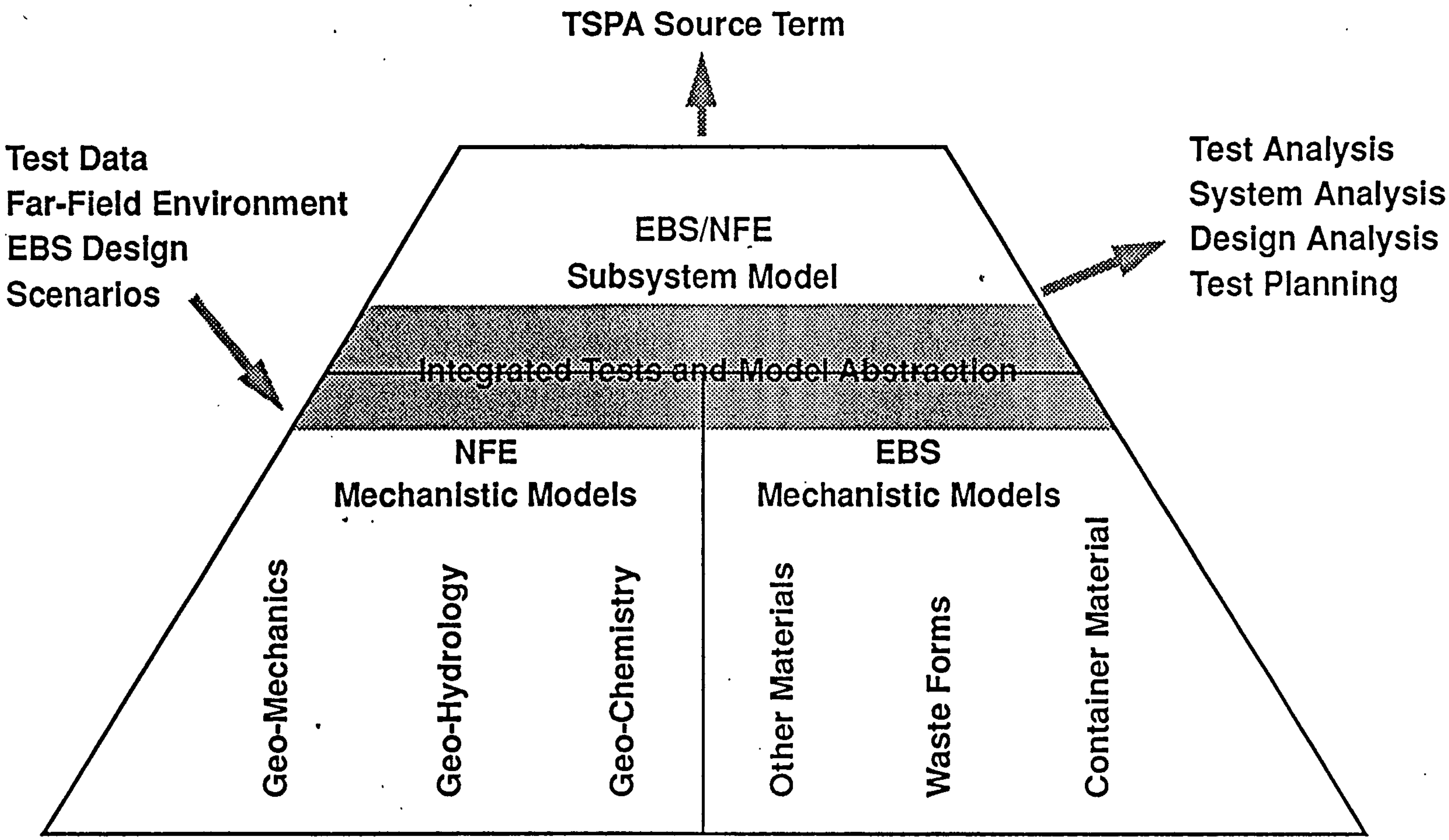
Waste Package Performance Modeling
- Design
- Near Field Environment
- Container
- Waste Form

Container Performance Models
- Oxidation
- General Aqueous Corrosion
- Localized Aqueous Corrosion

Iterative Interaction Between PA and Technical Program
- Subsystem Regulatory Compliance
- Testing and Model Development
- Design

Summary

EBS/NFE Subsystem PA Models



EBS Subsystem Modeling in TSPA-1993

YMIM (Yucca Mountain Integrating Model) was improved and modified to provide the source term for TSPA.

- A reduced version of YMIM was provided as a FORTRAN callable subroutine for the SNL-TSA package.

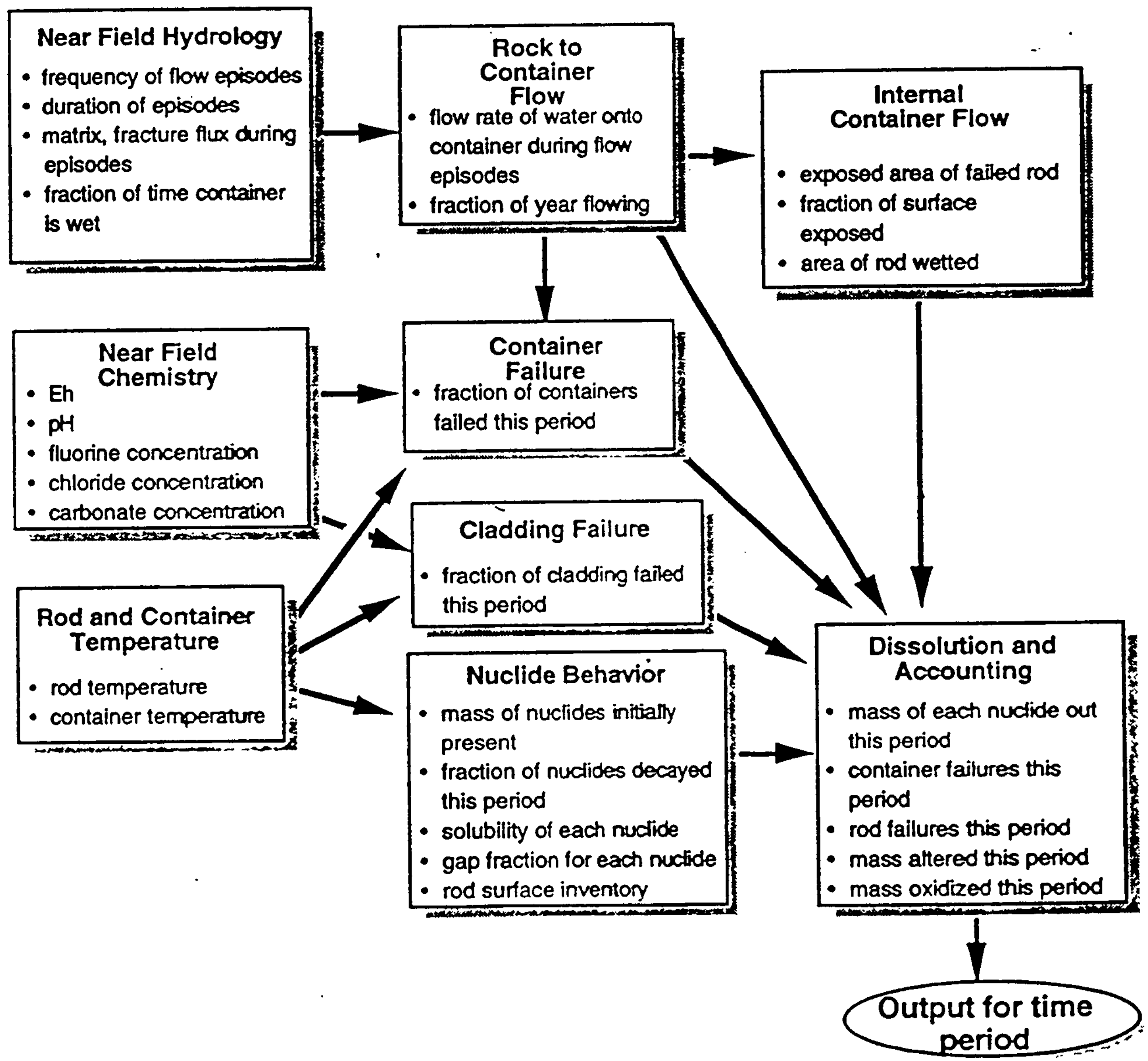
- The abstracted descriptions as incorporated in YMIM were provided to INTERA for use in the Golder-RIP model.

YMIM - Modular EBS/NFE model. Mechanistic container failure models for multiple degradation modes dependent on few group temperature, water contact and chemistry.

RIP - Deterministic WP model in a stochastic integrated system model. Few group representation of NFE and EBS. Container failure distributions specified for multiple degradation modes.

TSA - Package of codes (Total System Analyser) for probabilistic flow and transport analysis over a range of scenarios with an input source term.

Functional Structure of the YMIM Model



Current Developments (TSPA-1993)

TSPA-1 vs TSPA-1993

Feature/Process	TSPA-1 (1991)	TSPA-1993
Waste package	Small, thin wall	Small thin wall Large multiple material
Emplacement	Borehole	Borehole In drift
Thermal Loading	Implicit 57 kw/acre	Explicit: 28.5, 57, 114 kw/acre
Container performance	Arbitrary failure history Isothermal after 1000 yr.	Deterministic Temperature dependent Oxidation, General aqueous corr. Stochastic localized corrosion
Waste form performance	Isothermal, arbitrary rate	Temperature dependent Oxidation, Alteration, Dissolution
Near Field Environment	Isothermal, 'ambient'	Coupled hydrothermal modeling Temperature dependent Dry out effects Reflux effects

Preliminary Draft

Near Field Environment Modeling
(TSPA-1993)

- Temperature dependent.
- Water flow represents both ambient percolation flux and hydrothermally driven effects such as dry-out and refluxing.
- Abstracted from VTOUGH analyses for representative conditions.
- Few group representation of spatial variation from center to edge of repository. Log-normal representation of localized flux heterogeneity.
- Transient geochemical effects not currently incorporated.
- Effects of Man-Made Materials not currently incorporated.

Preliminary Draft

Dry Oxidation Modeling
(TSPA-1993)

- Dry oxidation rate extrapolated from high temperature data for iron and steel.

- Arrhenius temperature dependence.

- Primarily used for early time oxidation of thick steel overpack.

  • Key question: at what temperature-saturation conditions to switch to aqueous processes.

Example Dry Oxidation Data

$$\text{Rate} = Ke^{-k/T}$$

Temperature (°C)	Oxidation Rate (mm/yr)
Alloy 825[a]	
253	2.4×10^{-7}
20	5.5×10^{-16}
Carbon Steel[b]	
540	10.08
25	6.35×10^{-6}

[a] Data from Brasunas *et al.*, 1946

[b] Data from Uhlig, 1946

Aqueous General Corrosion Modeling

(TSPA-1993)

- Aqueous corrosion rate with a selectable pitting factor to represent localized rate variations.
- Selectable average rates, default values extracted from iron and steel corrosion data.
- Temperature relationship fitted to a quadratic shape with a maximum rate at a selectable temperature (such as 80°C).
- Primarily used for wet corrosion of thick steel overpack.

  • Key question: at what temperature-saturation conditions to switch to aqueous processes.

Example General Aqueous Corrosion Data

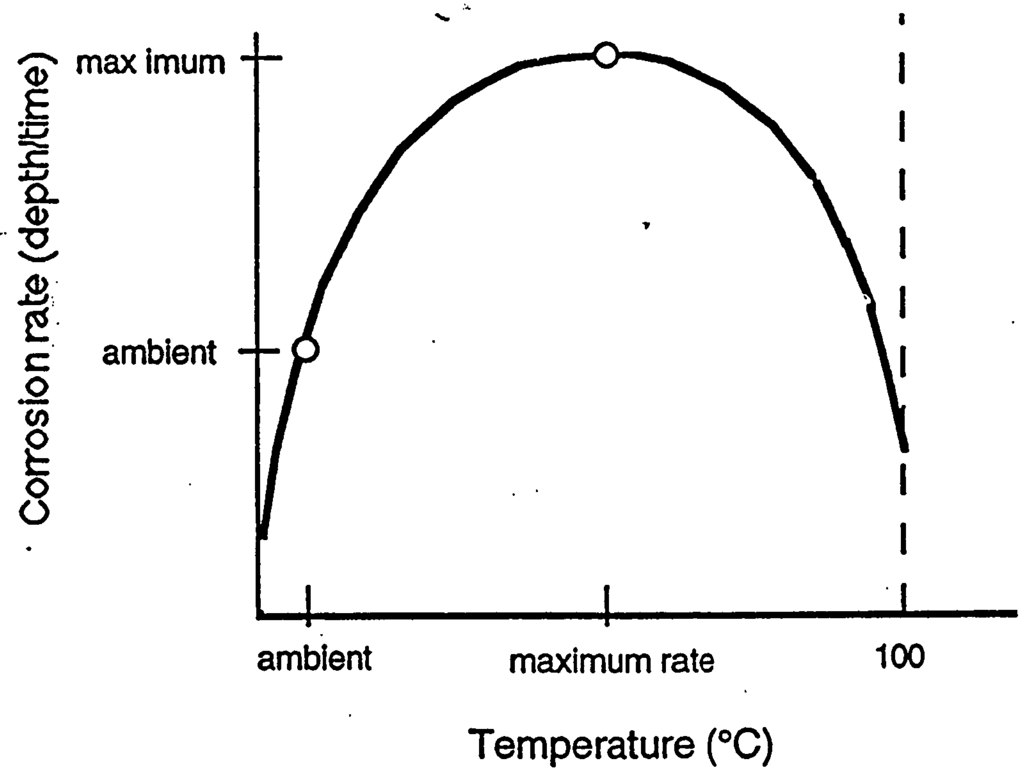


Figure 13-2. Generalized aqueous corrosion rate as a function of temperature.

Table 13-4. Generalized aqueous corrosion rates for mild steel.

Temperature (°C)	Rate (mm/yr)
80	0.38 (maximum)
20	0.12

Aqueous Localized Corrosion
(TSPA-1993)

- Combined representation of pitting and crevice corrosion.
- Abstracted from a stochastic pitting model (Henshall) which represents pit birth, growth and death probabilistically, with distributions normalized to fit pit depth data for austenitic corrosion resistant materials.
- Container failure time extracted via extreme value statistics over the active area of container surface.
- Temperature dependence fitted to an Arrhenius relationship of growth rate.
- Median, upper bound or lower bound growth rates selectable.

• Key question: at what temperature-saturation conditions to switch to aqueous processes.

Example Localized Aqueous Corrosion Data

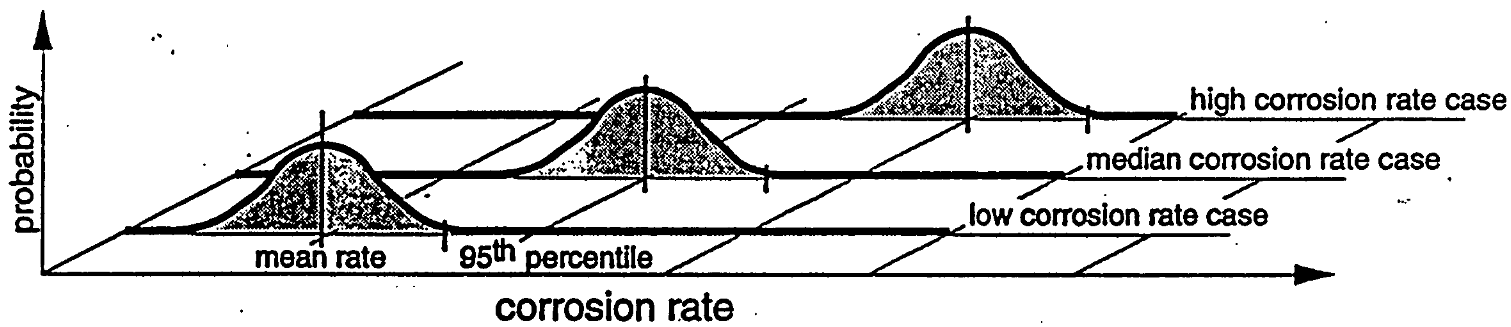


Figure 13-3. Illustration of pitting growth rates for 3 growth conditions.

Table 13-5. Estimates of stainless-steel corrosion rates.

	Temperature = 70°C		Temperature = 100°C	
Growth Condition	Mean Growth (mm/yr)	95th Percentile (mm/yr)	Mean Growth (mm/yr)	95th Percentile (mm/yr)
Low Growth Rate	0.0001	0.001	0.01	0.1
Median Growth Rate	0.001	0.01	0.1	1.0
High Growth Rate	0.01	0.1	1.0	10.0

Waste Package Lifetimes in TSPA-1993

Use of the YMIM corrosion models gave a range of WP lifetimes under different conditions:

- Waste Packages which were "wet" at near boiling temperatures failed in as little as 100 years.

- Waste Packages which stayed dry never failed in 1,000,000 years.

- Under evolving conditions most waste packages had lifetimes of several thousand years.

It should be noted that TSPA-1993 did <u>not</u> consider several potentially important effects:

- Delay of resaturation after temperatures dropped below boiling (extended dryout).
- Galvanic protection of the inner container by the outer.
- Microbiologically Influenced Corrosion.
- Effects of altered geochemistry.
- Effects of man-made materials.

Example Applications of EBS Subsystem PA to Design and Regulatory Compliance

An improved EBS/NFE model was developed to provide the TSPA-1993 source term.

- Interaction with the Waste Package ACD design team has begun. YMIM is available to the M&O (B&W) group to evaluate waste package design features, and to begin incorporation of improved design details into the model.

- The subsystem performance requirements were not addressed in TSPA-1993:
  - Substantially Complete Containment by the waste Package.
  - Controlled Release (10^{-5} of the 1,000 year inventory) by the EBS.

  Results may be extracted from the TSPA-1993 analysis. Additional analysis using YMIM and the TSPA scenarios will follow.

- Sensitivity/uncertainty studies have been started to assess the value of information in addressing design features, test planning and model development.

Example Application of EBS Subsystem PA Information Needs to Testing

Test data information needs were identified during development of the TSPA-1993 source term model:

- The transition of container corrosion mechanisms from non-aqueous to aqueous processes is important to understanding the effects of thermal loading and hydrothermal response on container lifetime. This transition is not currently understood adequately. Testing and model development were below the funding priority.

Test planning has been revised to address this issue:

- Controlled environment (temperature, humidity) corrosion experiments were elevated in priority as a result of PA input. Test plans have been prepared and thermogravimetric equipment procured. Preliminary test results will be available prior to the next TSPA.

Example Application of EBS Subsystem PA Information Needs to Model Development

Model development needs were identified during development of the TSPA-1993 source term model:

- Water contact with the waste package, driven or prevented by hydrothermal processes, may have significant impact on the source term. No suitable abstracted models exist.

Model development has been revised to address this issues:

- Abstracted models are being developed to describe reflux water flow and fracture flow penetration of dry rock both above and below boiling. Data extraction subroutines have been developed to allow hydrothermal flow time histories to be extracted from large volumes of modeling data.

Example Application of EBS Subsystem PA Information Needs to Site Testing

Model development needs were identified during development of the TSPA-1993 source term model:

- Water contact with the waste package, driven or prevented by hydrothermal processes, may have significant impact on the source term. Models and data of coupled processes are needed.

The Large Block Test at Fran Ridge is being adapted to address this issue.

- Material corrosion coupons will be incorporated to sample the hydrothermal environment.

- Environmental sensors are being incorporated to monitor the vapor phase air-water mixture and aqueous surface processes.

Summary

- Current EBS/NFE models are beginning to incorporate more mechanistic details such as hydrothermal water contact, temperature dependence, and specific corrosion processes.

- The primary purpose of these models is subsystem design and test analysis and to produce a source term for TSPA.

- Iterative interaction with design, testing, model development and TSPA is being actively pursued.

- More detailed EBS analysis will be possible in the future. Important developments will include: waste package design details, container material specification, improved mechanistic models and improved definition of the near-field environment such as water contact, geochemistry and man-made materials.