Uncertainty Characterization and Model Integration:

An Example from the Yucca Mountain License Application

DOE-EM Performance Assessment Community of Practice Technical Exchange Meeting

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Salt Lake City, UT

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Sandia National Laboratories

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NNSA National Nuclear Security Administration

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Presentation Outline

- Major steps in a Performance Assessment (PA)
- Integration of process models and abstractions into the PA
- Process for characterizing uncertainty and variability in key inputs, and ensuring consistency among models
- Construction of the system model and analyses as a function of uncertainty
- Uncertainty and sensitivity analyses: feedback regarding the key uncertain parameters

Major Steps in a Performance Assessment

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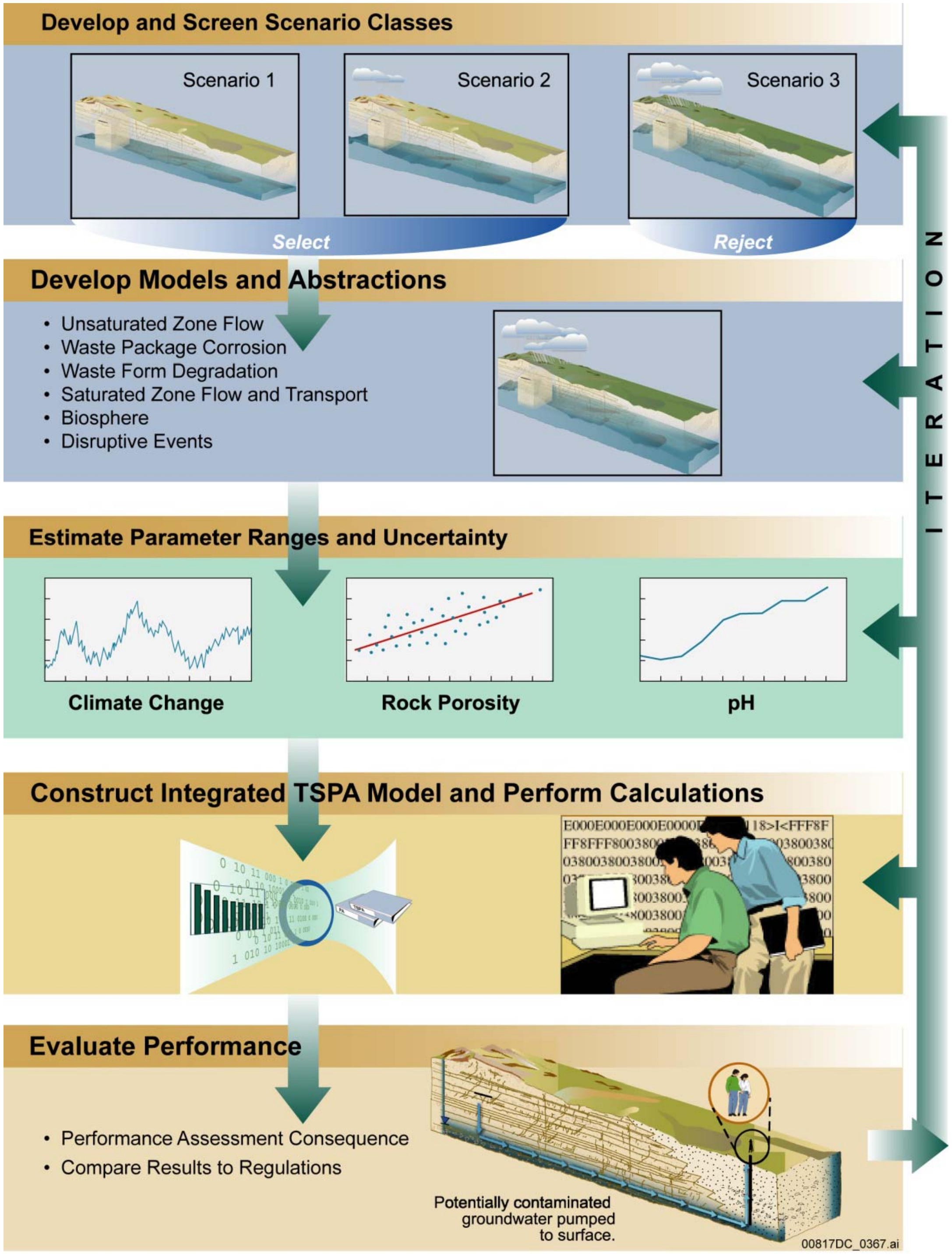
Major Steps in a Performance Assessment

- **Select (and screen) Features, Events, and Processes (FEPS) and develop scenario classes**
- **Develop process models (and, perhaps, abstractions or reduced-order models), along with their scientific basis**
- **Evaluate parameter and model uncertainty**
- **Construct integrated system model with a consistent treatment of uncertainty**
- **Evaluate system model results, including the effects of uncertainty (conduct uncertainty/sensitivity analyses)**
- **Iterate**



History of DOE Yucca Mountain Total System Performance Assessments (TSPAs)

(from http://www.nwtrb.gov/meetings/2004/sept/04sept.html)

TSPA Iteration	Summary of Key Results
1988 Site Characterization Plan	• Applied basic methodology for Monte Carlo uncertainty analyses based on scenarios.
TSPA-1991	• Demonstration of TSPA approach. • Models limited to UZ and SZ, and volcanism identified importance of uncertainty in UZ flow paths.
TSPA-1993	• Improved models for UZ, SZ, early models for coupled processes, EBS, biosphere. • Importance of uncertainty in thermal hydrology, UZ flow, corrosion of engineered materials.
TSPA-1995	• Incorporate new science and design, evaluate alternative models. • Importance of robust process models for WP degradation, seepage, UZ and SZ transport.
TSPA-VA	• Supported the 1998 Viability Assessment, models based on best current information. • Ranked importance of uncertainty in each of the major components for 10,000, 100,000, and 1,000,000 years. • Emphasis on seepage, water chemistry, corrosion, and SZ.
1999 License Application Design Selection (LADS)	• TSPA tools used to evaluate relative merits of design alternatives. • Demonstrated that multiple designs were viable for long-term performance.
TSPA for Site Recommendation (2000)	• Robust modeling system using fully qualified inputs • Conservative approach to some components. • Regulatory importance of volcanism identified. • Conservative treatments of uncertainty complicated realistic understanding.
FY 2001 Supplemental Science and Performance Analyses (SSPA)	• More realistic treatment of uncertainty. • Incorporation of new information since TSPA-SR. • Confirmed potential suitability. • Confirmed importance of volcanism and EBS performance for 10,000 years. • Insights into EBS and natural system effects on peak dose.
TSPA for the Final Environmental Impact Statement (2001)	• Updated SSPA to include new information, revised regulatory boundary.
2002 Sensitivity Analyses (one-on and one-off)	• Insight into barrier performance. • Risk-importance information regarding model components. • Importance of volcanic disruption for 10,000-yr regulatory compliance.
TSPA-LA	• Models updated to current information.

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Major Steps in a Performance Assessment

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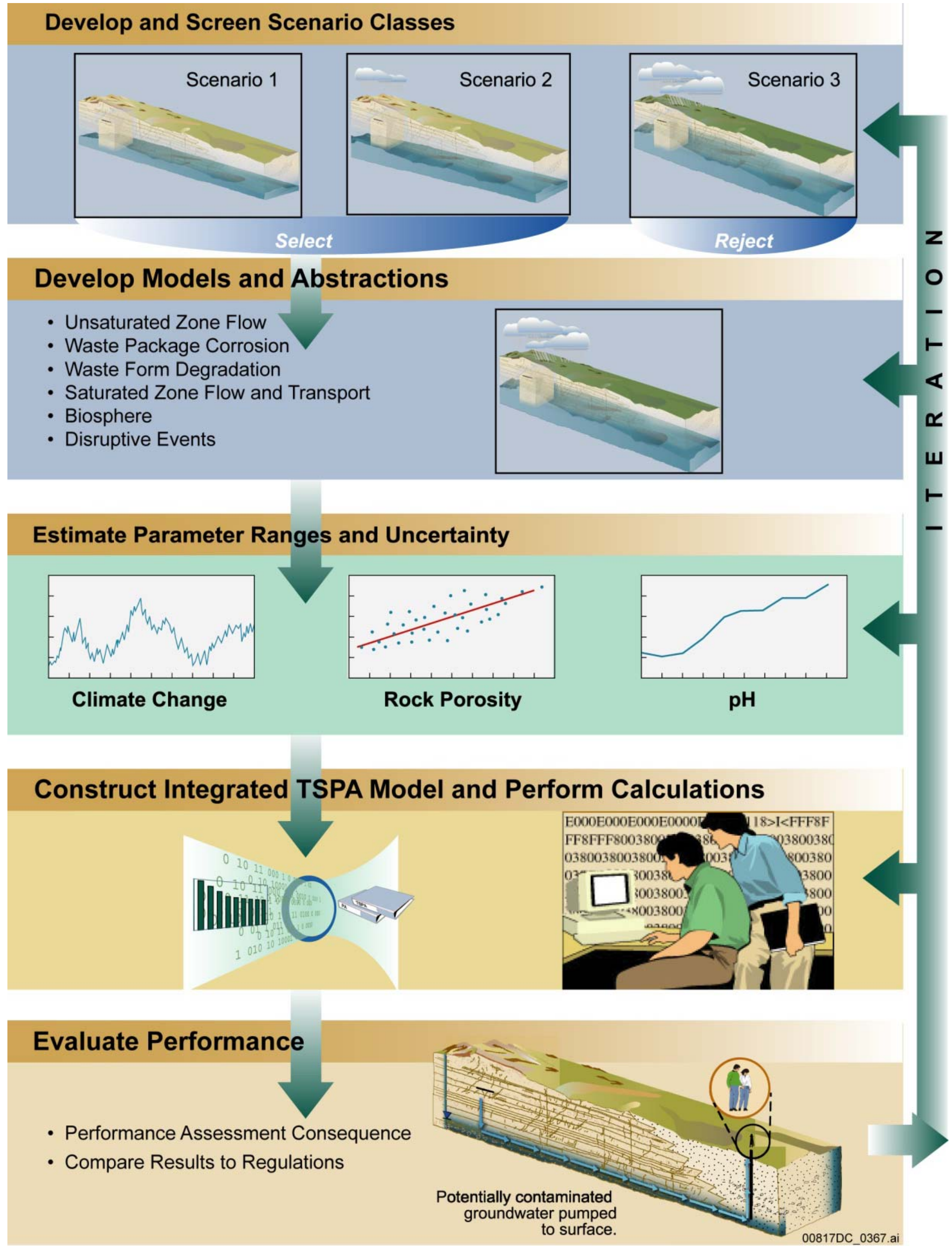


Construct and Screen Scenario Classes

Future Scenarios for Yucca Mountain

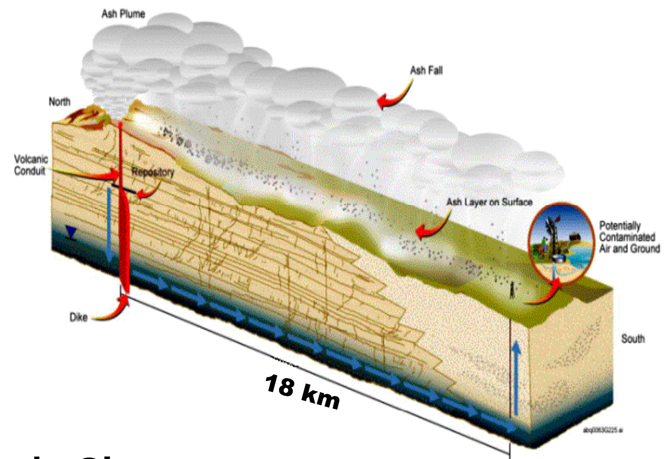
- **Four scenario classes divided into seven modeling cases**

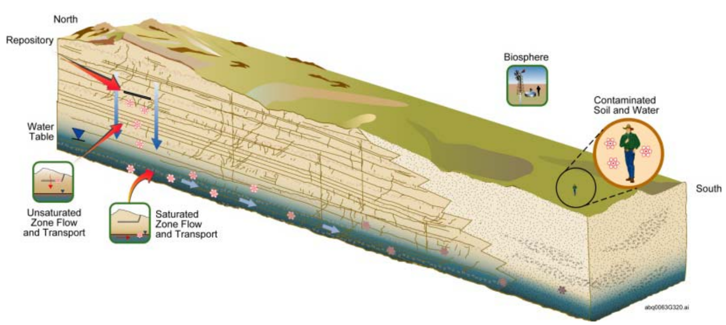
  - **<u>Nominal Scenario Class</u>**
    - **Nominal Modeling Case (reference state)**

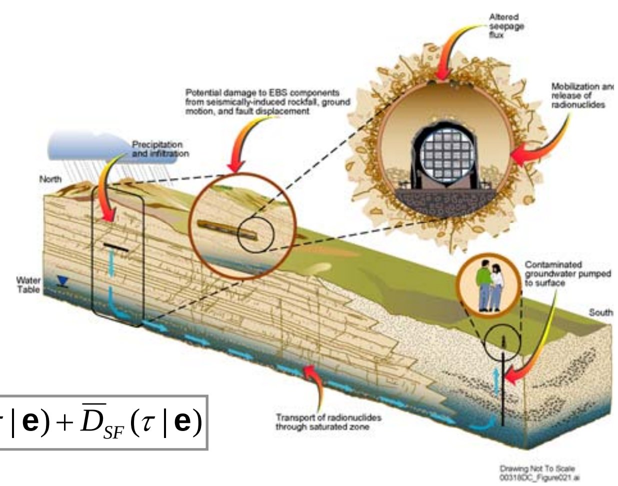
  - **<u>Early Failure Scenario Class</u>**
    - **Waste Package Modeling Case**
    - **Drip Shield Modeling Case**

  - **<u>Igneous Scenario Class</u>**
    - **Intrusion Modeling Case**
    - **Eruption Modeling Case**

  - **<u>Seismic Scenario Class</u>**
    - **Ground Motion Modeling Case**
    - **Fault Displacement Modeling Case**



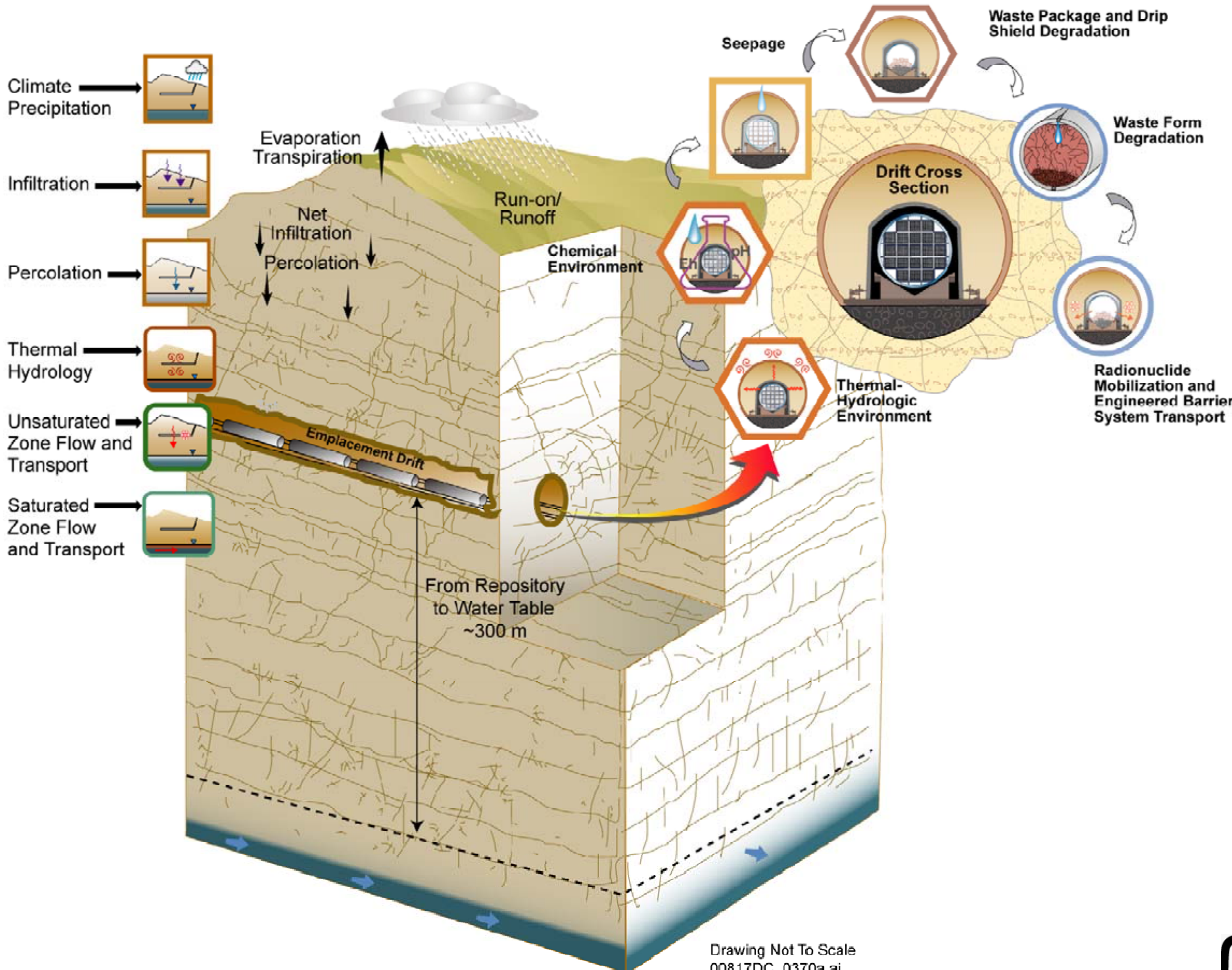




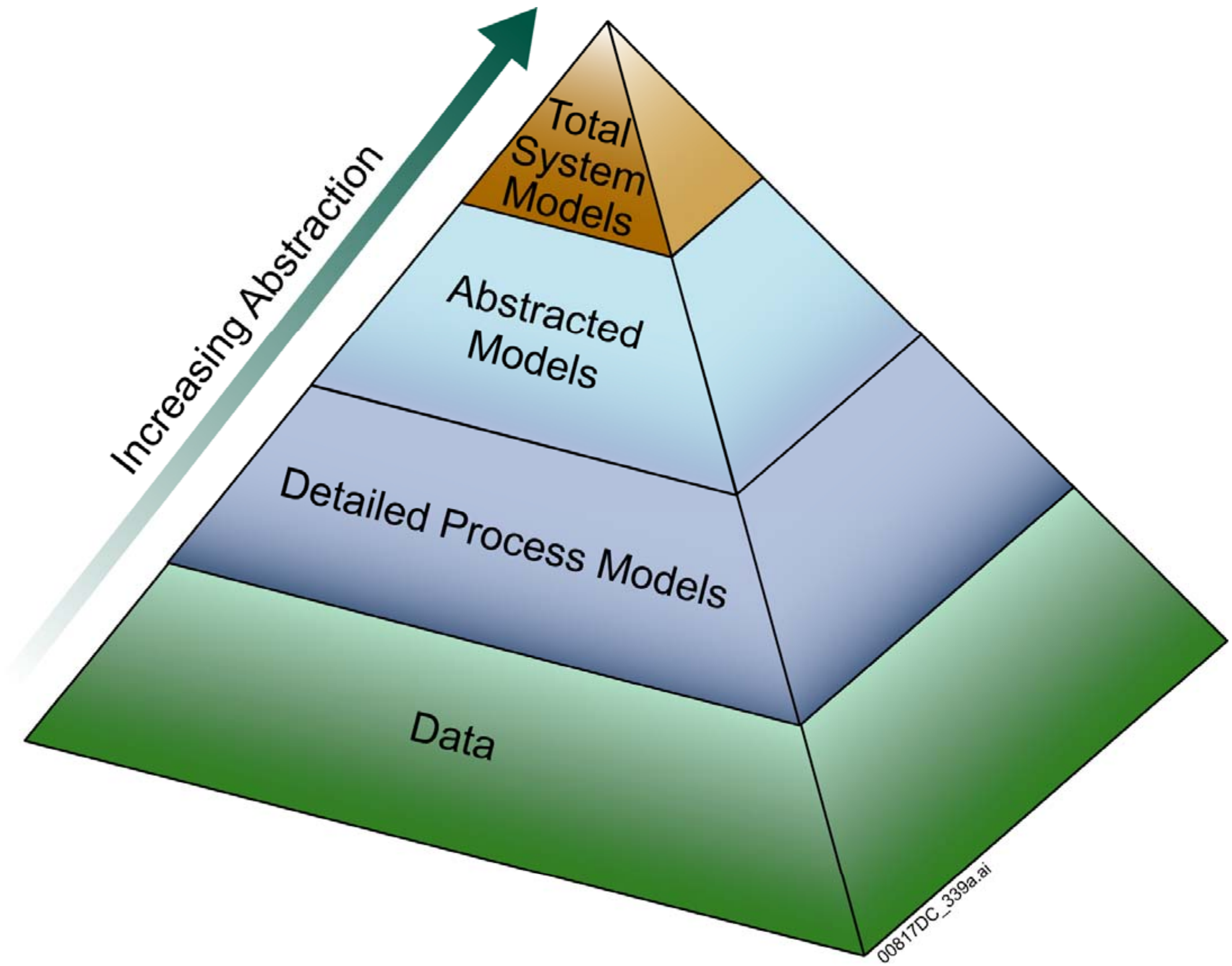
$$\overline{D}(\tau|\mathbf{e}) \cong \overline{D}_N(\tau|\mathbf{e}) + \overline{D}_{EW}(\tau|\mathbf{e}) + \overline{D}_{ED}(\tau|\mathbf{e}) + \overline{D}_{II}(\tau|\mathbf{e}) + \overline{D}_{VE}(\tau|\mathbf{e}) + \overline{D}_{SG}(\tau|\mathbf{e}) + \overline{D}_{SF}(\tau|\mathbf{e})$$

Develop Process Models and Abstractions

Expected Processes for the Natural and Engineered Barrier Systems at Yucca Mountain

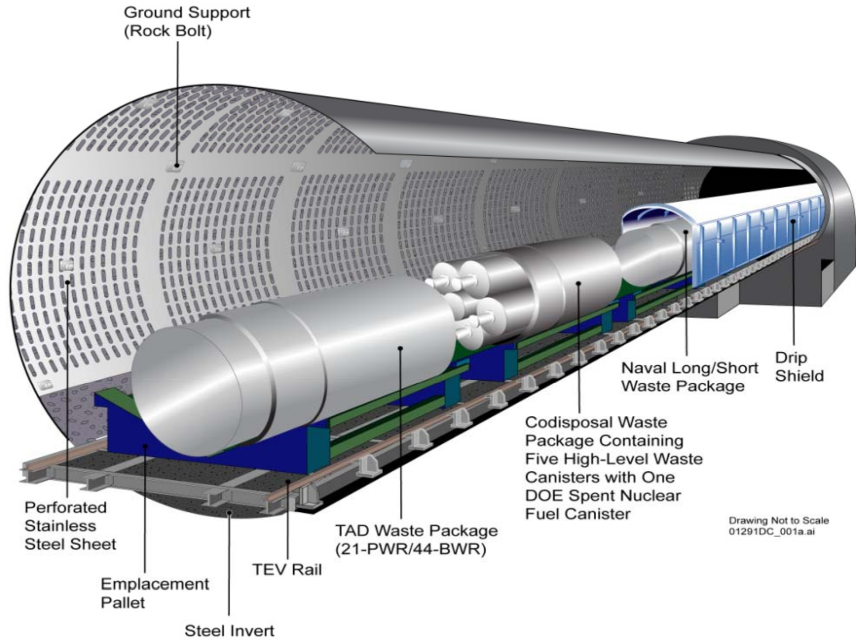


Construct Integrated System Model

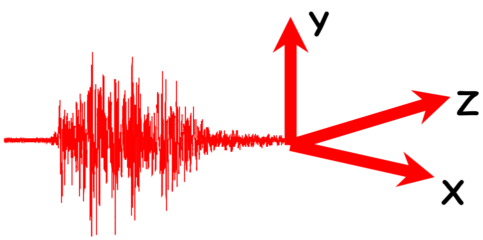


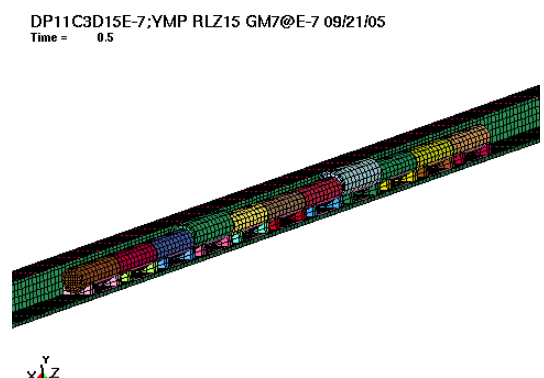
Process Model: Seismic Ground Motion in Intact Drifts

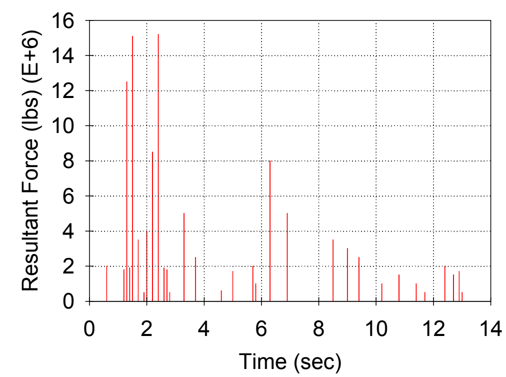
- **3-D kinematic analyses (using LS-DYNA code) of CSNF and co-disposal WPs, to produce histories of multiple WP impacts for each of 17 ground motion time histories at four horizontal PGV levels**



Schematic Ground Motion Time History → **Representative Drift Configuration** → **Illustrative Impact Force History**

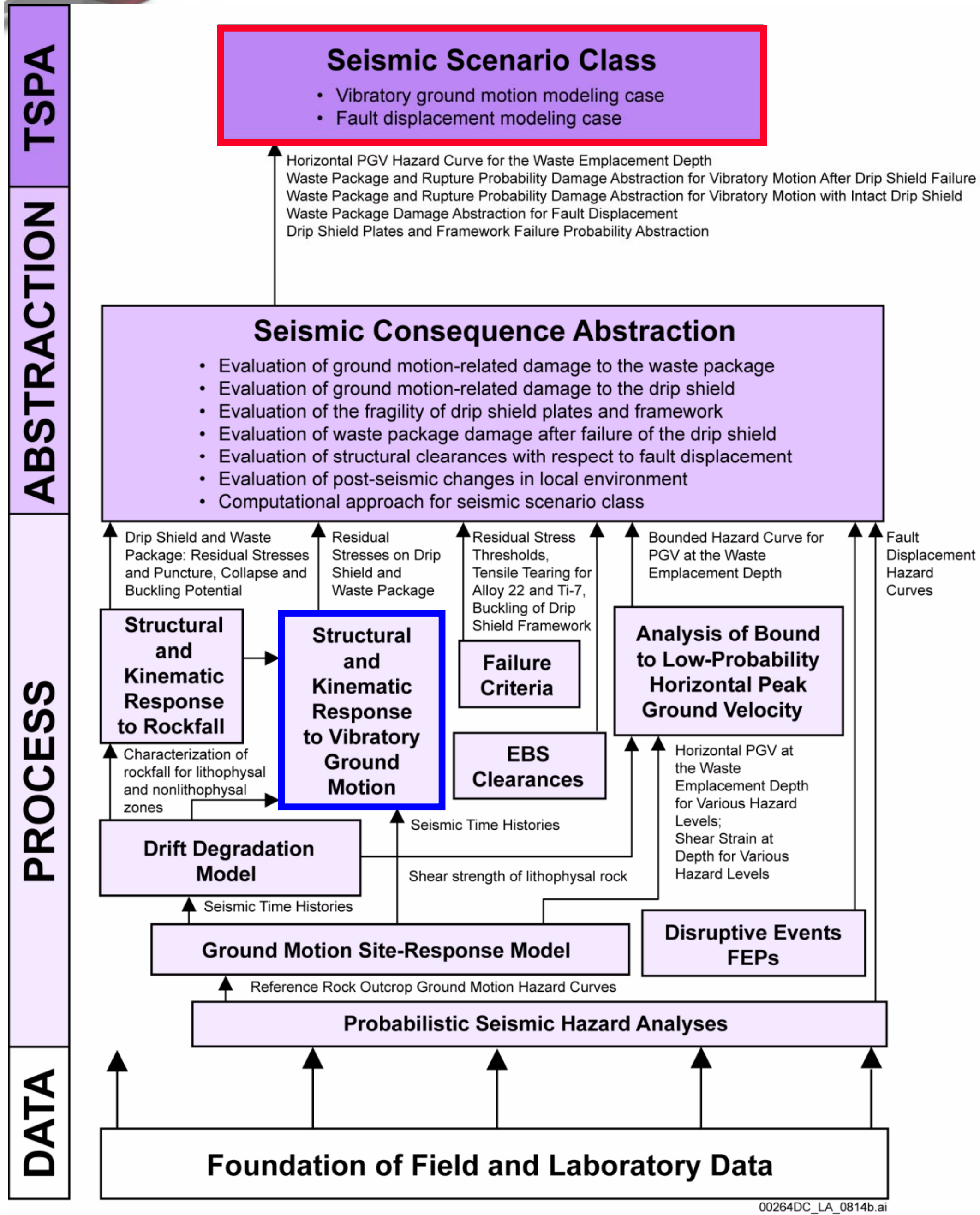


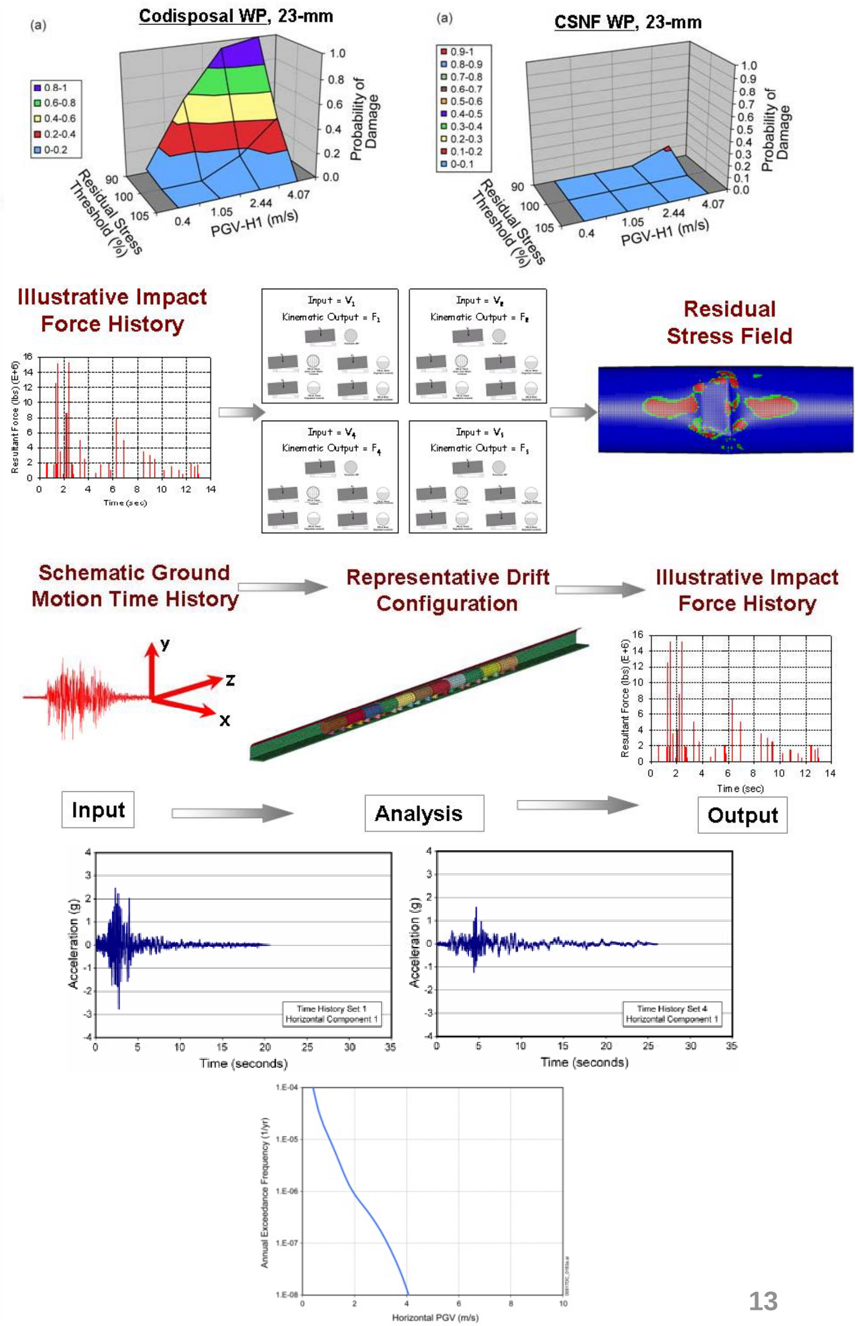




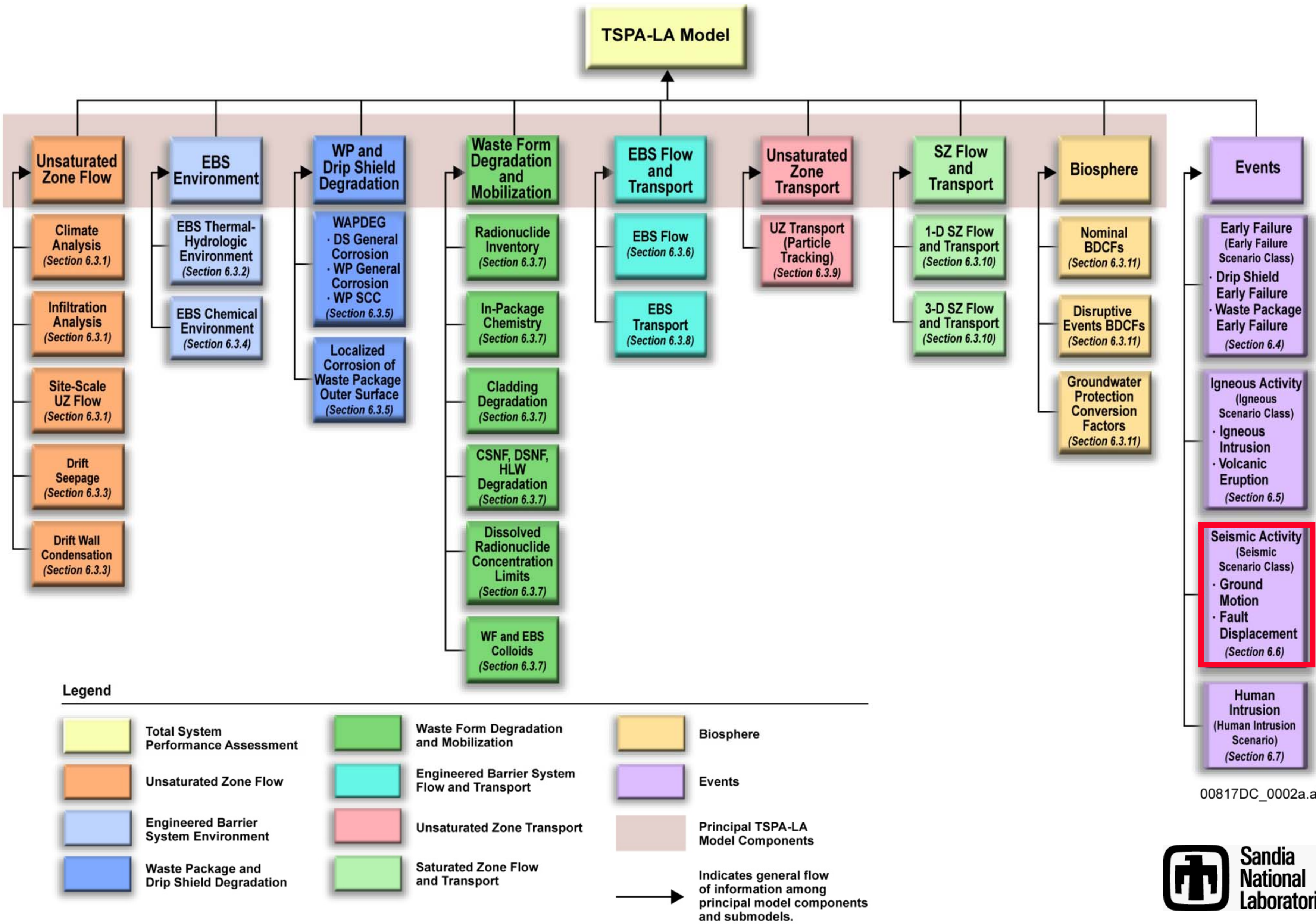
Input → **Analysis** → **Output**

Incorporation of Seismic Effects in the PA





Performance Assessment System Model
(and component models and submodels)



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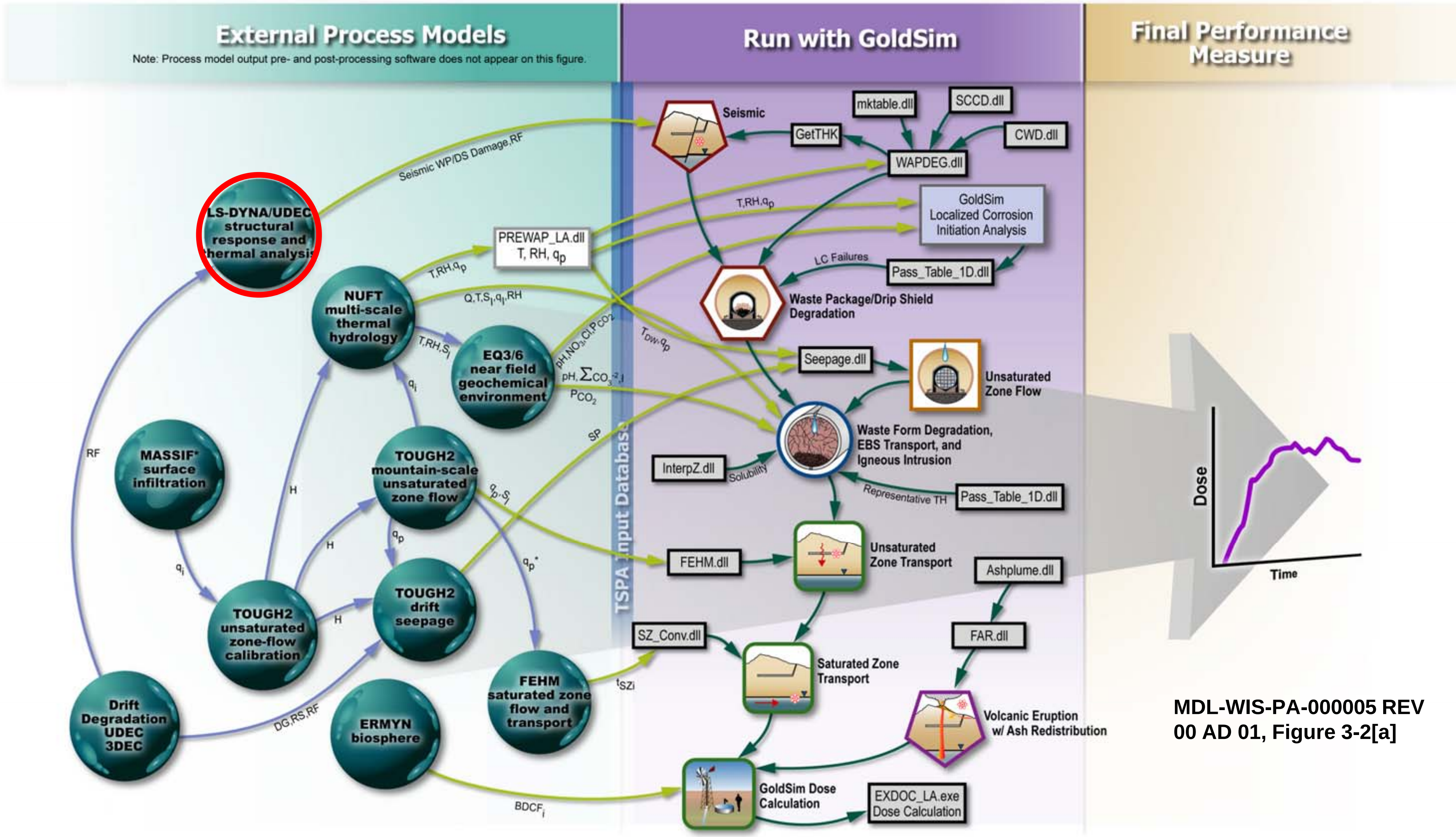
YM Software Architecture



MDL-WIS-PA-000005 REV 00 AD 01, Figure 3-2[a]

Output Parameters

f_S	Fraction of WPs with Seeps	q_p	Percolation Flux	q_i	Infiltration Flux	H	Hydrologic Properties
EBS	Engineered Barrier System	NO_3	Nitrate Concentration	DG	Drift Geometry	SP	Seepage Parameters
Q_S	Seep Flow Rate	T	Temperature	Cl	Chloride Concentration	RS	Rock Strength
Q	Evaporation Rate	RH	Relative Humidity	I	Ionic Strength	RF	Rockfall Size and Number
pH	pH	S_l	Liquid Saturation	t_{SZi}	Saturated Zone Transport Time		
ΣCO_3^{-2}	Carbonate Concentration	X_a	Air Mass Fraction	$BDCF_i$	Biosphere Dose Conversion Factor		
P_{CO_2}	Partial Pressure of CO_2	q_l	Liquid Flux	q_g	Gas Flux	*Note: q_p derived from INFIL model	

Legend

- Response Surface between Process Models
- Response Surface from Process Model to GoldSim
- Connection in GoldSim
- Preprocessor
- TSPA Model DLL

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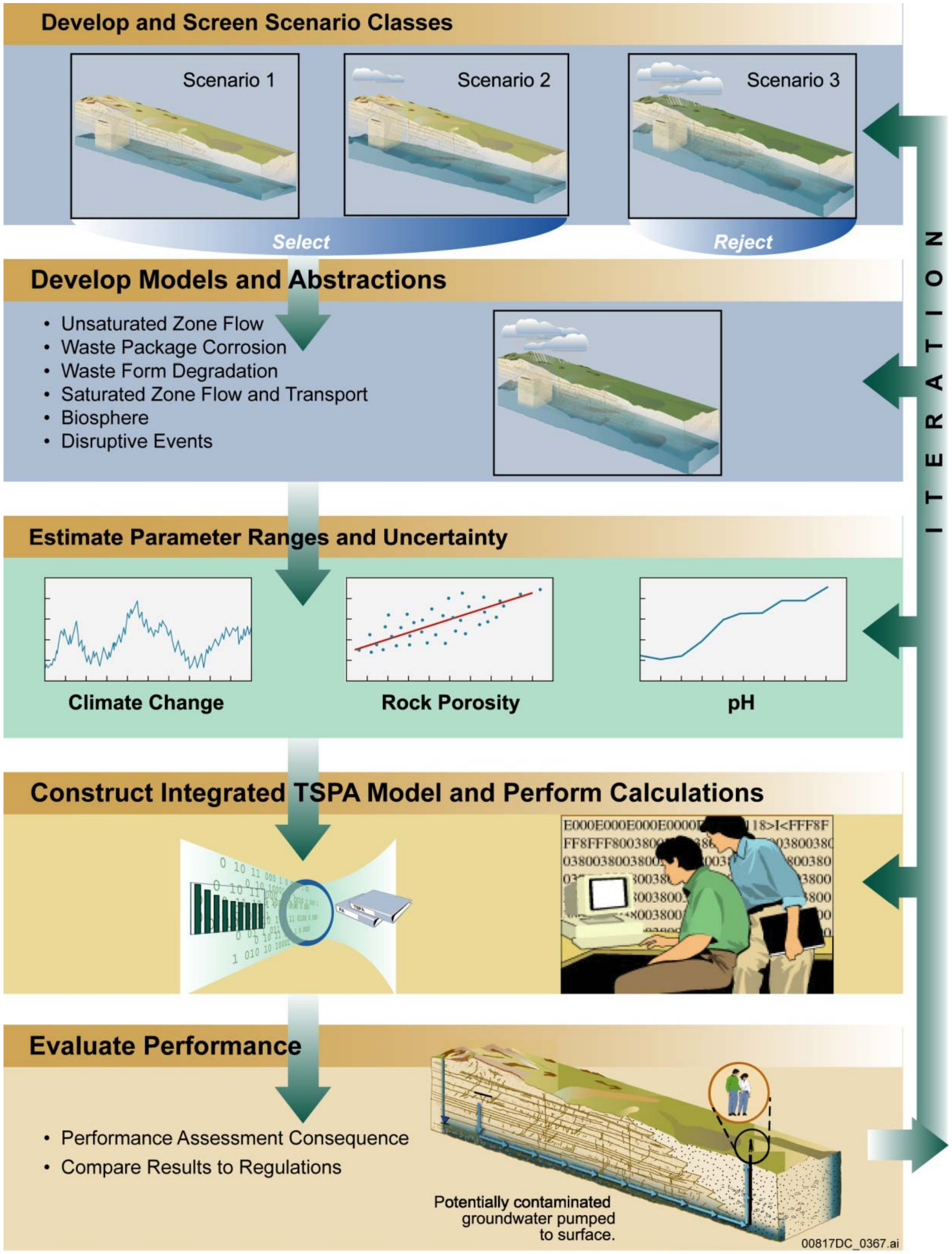


Evaluate Parameter and Model Uncertainty

- **Sources and Types of Uncertainty**
- **A Process for Consistent Characterization of Uncertainty and Variability**
- **Developing Input Parameter Uncertainty Distributions**

Sources and Types of Uncertainty (Uncertainty Classification)

- Parameter Uncertainty
- Conceptual Model Uncertainty
- Scenario Uncertainty

Major Types of Parameter Uncertainty

Aleatory Uncertainty

- Inherent randomness in events that could occur in the future; cannot be reduced by further measurements
- Alternative descriptors: irreducible, stochastic, intrinsic, type A
- Examples:
  - *Time and size of a seismic event (time = hazard curve; size = ground motion time history)*
  - *Damage caused by seismic event*

Epistemic Uncertainty

- Lack of knowledge (or degree of belief) about appropriate value to use for a quantity assumed to have a fixed value; can be reduced by further measurements (feedback for prioritizing experimental program)
- Alternative descriptors: reducible, subjective, state of knowledge, type B
- Examples:
  - *Waste-form degradation rates, chemical equilibrium constants, sorption coefficients, inventory masses, corrosion rates, etc.*
  - *Rates defining Poisson processes*

Evaluate Parameter and Model Uncertainty

- **Sources and Types of Uncertainty**
- **Consistent Characterization of Uncertainty and Variability across all Models**
- **Developing Input Parameter Uncertainty Distributions**

Uncertainty and Variability Characterization Review Process

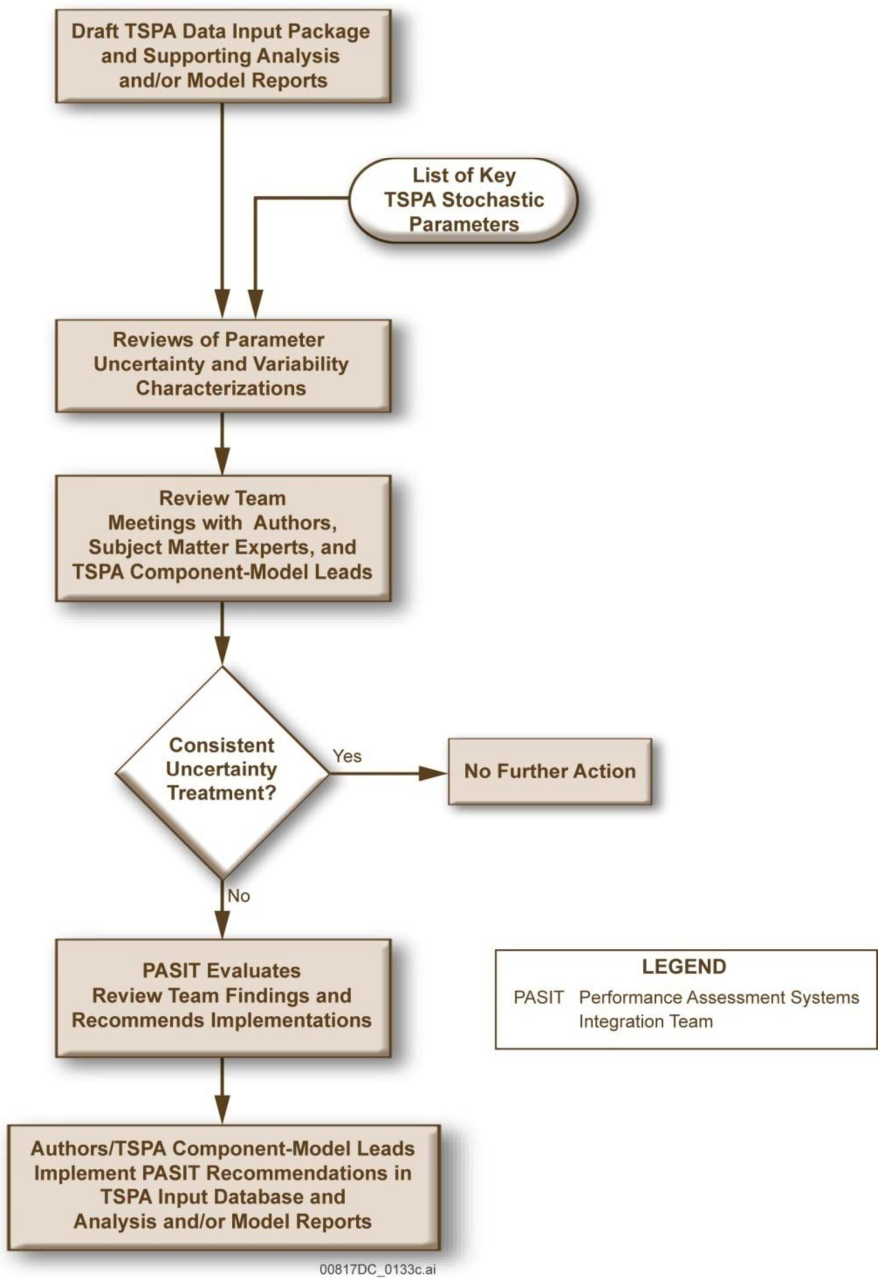
- **Parameter uncertainty review team (PUT):**
  - Senior staff members (~ 5 or 6) with expertise in (1) probabilistic modeling and uncertainty propagation, (2) statistical analysis of field and laboratory data, (3) sensitivity and uncertainty analysis, (4) use of expert judgment to inform distribution construction, and (5) total system modeling for the particular system of interest
  - PUT workscope:
    - Familiarize subject matter experts (SMEs) with methodologies for analyzing uncertainty and variability, as well as the use of statistical techniques for deriving probability distributions
    - Perform independent statistical analyses of available data
    - Help SMEs derive probability distributions using advanced techniques
    - Examine subjective probability distributions to ensure that professional judgment was incorporated in a reasonable fashion

Risk-Informed Identification of Key Uncertain Parameters

- **Selection of review parameters is an iterative process based on:**
  - **risk-informed ranking of key models, processes, and scenario classes**
  - **uncertainty and sensitivity analyses conducted during model development or prior iterations**
  - **recommendations of SMEs**
- **<u>Note</u>: it is not necessary to treat all parameters as uncertain; reduce this set based on prior analyses**

PUT Parameter Review Process

- Review relevant source documents
- Meetings with authors, data collectors, SMEs, and analysts
- Develop recommendations and/or independent probabilistic representations
- Present findings and recommendations to SMEs and appropriate technical management
- If necessary, a senior technical management team decides on the appropriate uncertainty implementation, based on a risk-informed perspective



Multiple Institutions Involved in the Uncertainty Characterization and Model Integration Process

- **Lead Lab (Sandia)**
- **Interfaces / Teammates:**
  - **Multiple National Labs**
  - **Universities, Consultants**
  - **Subcontractors**
    - **Services and Staff Aug**

Evaluate Parameter and Model Uncertainty

- **Sources and Types of Uncertainty**
- **Consistent Characterization of Uncertainty and Variability**
- **Developing Input Parameter Uncertainty Distributions**

Parameter Uncertainty Estimation Workshop
(Common Ground for the Technical Staff)

- **Project-wide parameter uncertainty workshop convened early in the process to put all technical staff on a common ground with respect to parameter characterization and the associated review process**

- **Example topics discussed at workshop:**
  - Nature and sources of uncertainty
  - Fitting continuous distributions
  - Fitting distributions to small samples
  - Subjective assessment of probabilities
  - Bayesian updating
  - Scaling issues
  - Model uncertainty

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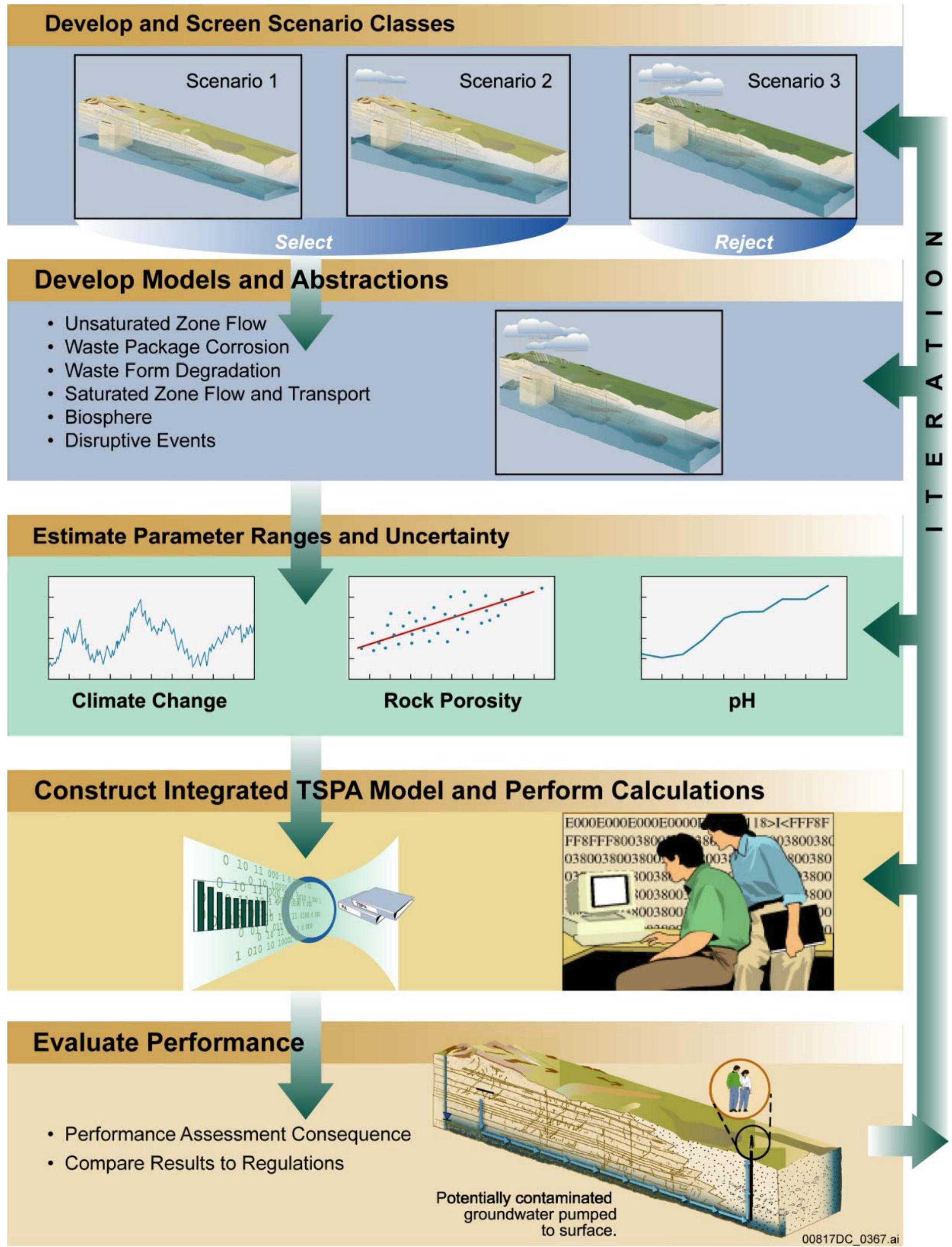


Uncertainty and Sensitivity Analyses:

With an Example from Yucca Mountain

Basic Parts of Analysis

- Characterization of aleatory uncertainty in occurrence of future events
  - **a** = [a_1,a_2,…] vector characterizing a possible future at YM site
    - ➢ *e.g.,* $\mathbf{a} = [nSG, t_1, v_1, t_2, v_2, \cdots, t_{nSG}, v_{nSG}]$ *for seismic ground motion events in time interval* [*0 , 10*^{4} *yr*], *where* nSG= *number of seismic events,* t_i = *time* (*yr*) *of* i^{th} *event, and* v_i = *PGV (peak ground velocity) for* i^{th} *event*

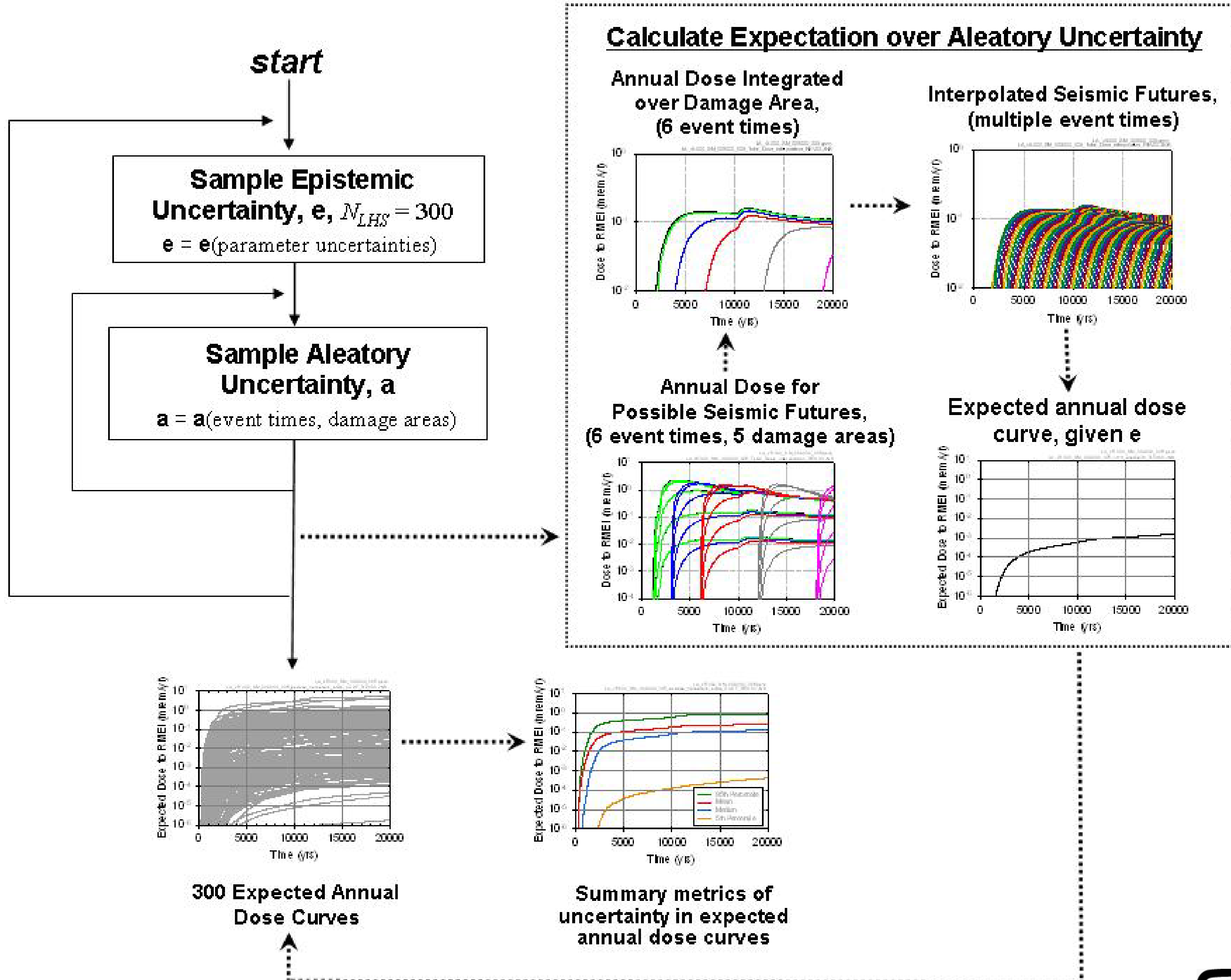
- Characterization of epistemic uncertainty in analysis inputs
  - **e** = [e_1,e_2,…,e_{nE}] vector of epistemic uncertainty in TSPA inputs
    - ➢ e.g., uncertainty in corrosion rates, degradation rates, radionuclide solubilities, etc.

- Models for predicting the physical behavior and evolution of the repository
  - Function **y** = **f**(**e**), where **y** is a vector of epistemically uncertain TSPA outputs, dependent on the epistemically uncertain inputs **e**; and **f** is the suite of models constituting the TSPA
  - **y** has many components, e.g., receptor dose; releases from the EBS, unsaturated zone, saturated zone; chemical conditions in the EBS; etc.

Analysis Approach

- Define distributions for the set of N_E epistemically uncertain input parameters ($N_E \cong 400$ for Y.M.)
- Generate Latin Hypercube Sample (LHS) $\mathbf{e}_i = [e_{1i}, e_{2i},\ldots e_{NEi}]$, $i=1,2,\ldots,N_{LHS}$, consistent with defining distributions (N_{LHS} = 300 for Y.M.)
- Evaluate $\mathbf{y}_i = \mathbf{f}(\mathbf{e}_i)$, $i=1,2,\ldots, N_{LHS}$, for each LHS element i
- Present uncertainty results: Cumulative and complementary cumulative distribution functions (CDFs, CCDFs), quantiles, expected values, …
- Perform sensitivity analysis on mapping $[\mathbf{e}_i, \mathbf{y}_i(\mathbf{e}_i)]$, $i=1,2,\ldots,N_{LHS}$: scatterplots, partial rank correlation coefficients (PRCCs), stepwise rank regressions, …

Calculation Methodology for Seismic Expected Dose



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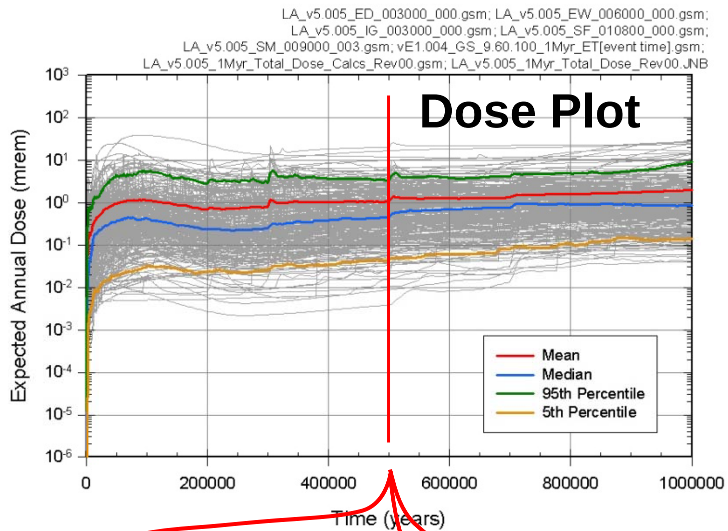
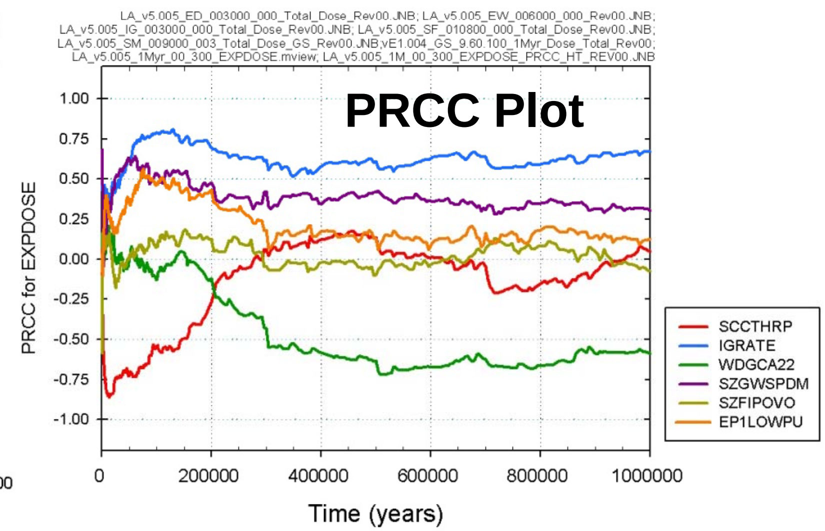
Uncertainty in Total Expected Dose:
(Sum over All Scenario Classes and RNs)

SCCTHRP – Stress threshold for SCC initiation

IGRATE – Frequency of igneous events

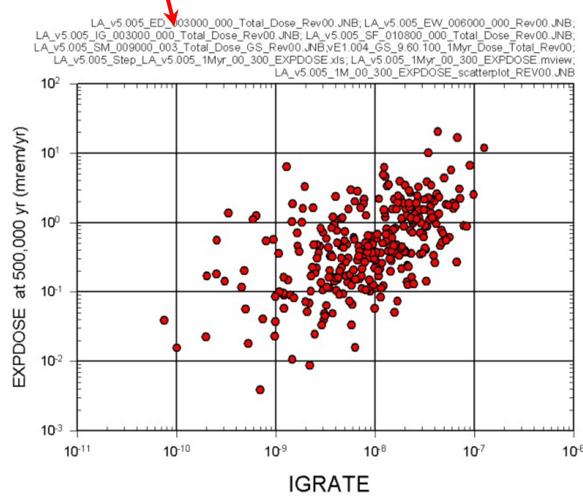
WDGCA22 – Temperature dependence in A22 corrosion rate

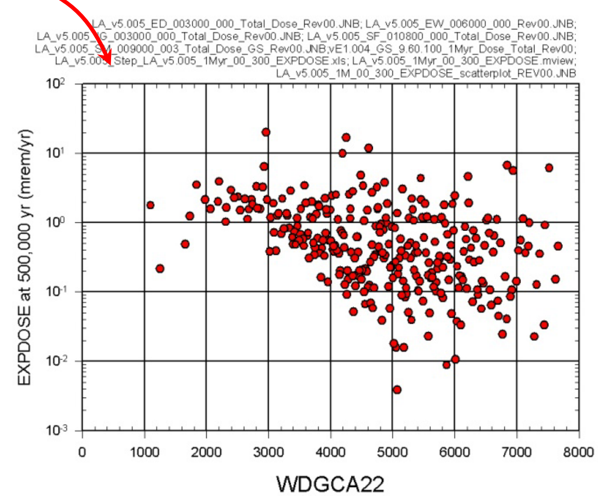




Linear Regression

EXPDOSE: 500,000 Years		
Variable	R^2	SRRC
IGRATE	0.29	0.54
WDGCA22	0.46	−0.38
SZGWSPDM	0.53	0.24
EP1LOWNU	0.56	0.19
MICNP237	0.59	0.16
EP1L0WPU	0.61	0.17
SZCONCOL	0.64	0.15
SZFISPVO	0.66	0.15
INFIL	0.67	0.11
GOESITED	0.68	−0.10
SZKDCSVO	0.69	−0.10
HFOSITED	0.69	−0.09
SZDIFCVO	0.70	−0.09





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Summary

- **Uncertainty is an important component of the analysis of any complex system and needs to be addressed accordingly**
- **A systematic approach to performance assessment, uncertainty characterization, and uncertainty/ sensitivity analysis is beneficial:**
  - **Enhances transparency, consistency, as well as credibility with regulator**
  - **Provides a probability or confidence level to the possible outcomes**
  - **Provides valuable insights as to which parameters are most important**
- **Where does each process model fit into the safety assessment?**
  - **Use a risk-informed approach to determine the level of importance of various parameters and models**
  - **Expend more effort on characterizing key uncertain parameters**

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Summary (continued)

- **Every scientific group (data, models, computational, etc.) has a role in ensuring a consistent and reasonable treatment of uncertainty**
  - **Communication is essential between the groups**
  - **Document your decisions and provide the rationale**
- **The process is iterative—new data, analyses, and understanding will lead to future refinements. However, uncertainty and sensitivity analyses will help determine the areas that need study/ improvement**

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Nuclear Energy Advanced Modeling & Simulation (NEAMS)

Waste Forms & Systems Integrated Performance & Safety Code System

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April 15, 2009

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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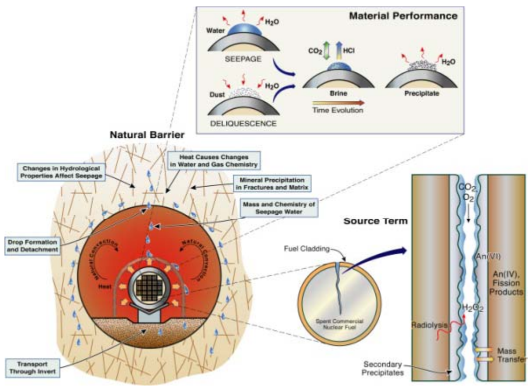
NEAMS Program Strategy –
Waste Forms & Systems IPSC



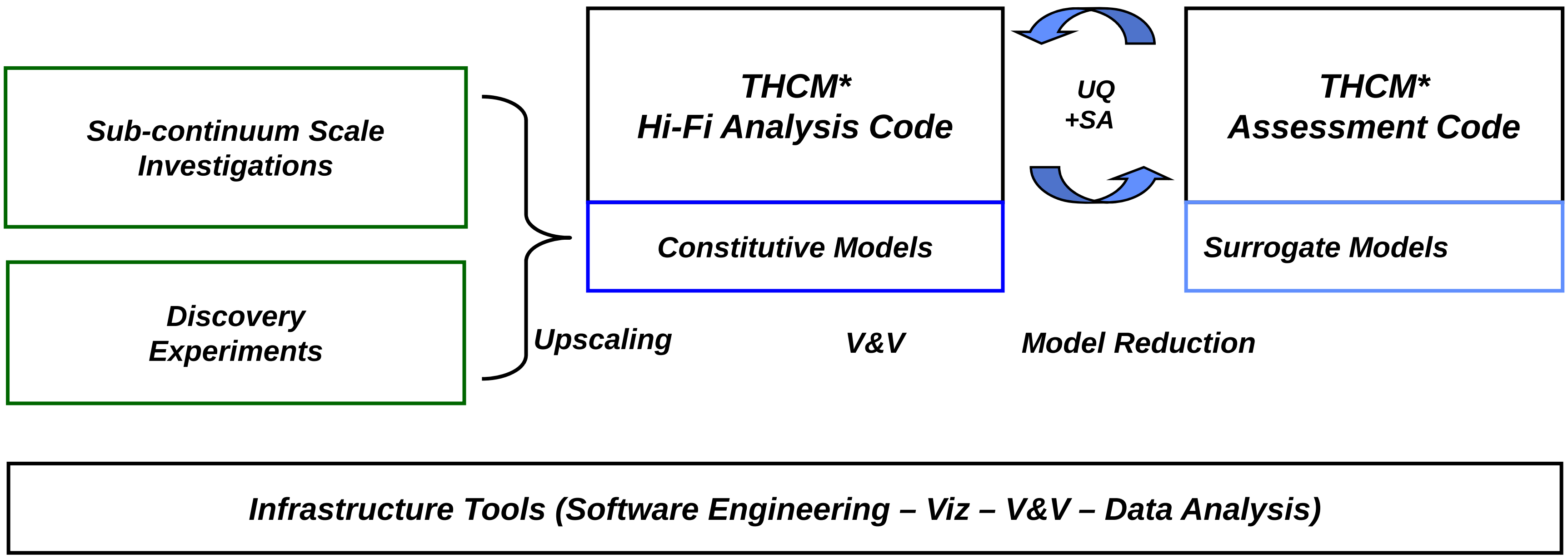
Strategy Vision

As an integral part of nuclear energy generation and management, we will develop an integrated, science-based simulation package for assessing performance of potential nuclear reactor waste storage or disposal options, from the waste form itself through the entire surrounding engineered environment and representing the range of important multi-scale effects.

Milestones

- **Years 0-3:**
  - IPSC Design Specifications
  - PIRT & V&V Plan
  - THCM Architecture and Prototype
  - High priority sub-continuum studies
  - Generation of constitutive models
  - Initial Demonstration to WF/Environment Reference Case
- **Years 4-10**
  - High-fidelity continuum and surrogate models
  - Initial release of THCM and Assessment Codes
  - Full application to WF/repository environment

WF IPSC Relationships



*** THCM:** ***T**hermal/**H**ydrological/**C**hemical/**M**echanical*