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NEAMS VU ELEMENT

An Improved Best Estimate Plus Uncertainty Methodology Including Advanced Validation Concepts to License Evolving Nuclear Reactors

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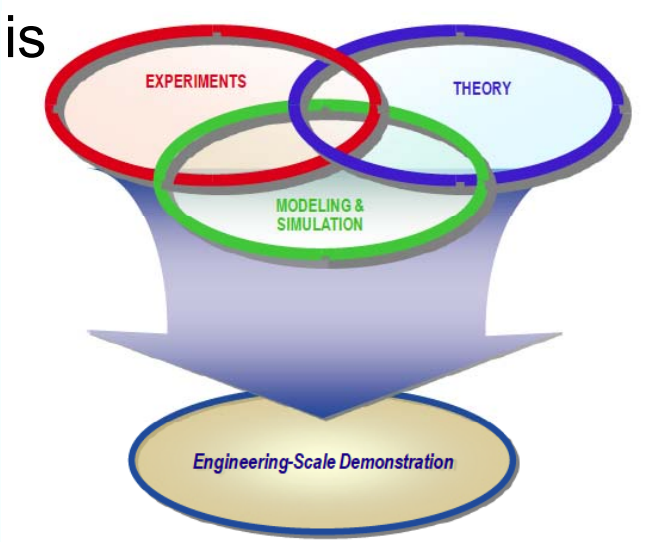
Outline

- Objectives
- Current Regulatory Process & CSAU Overview
- Challenges to Licensing Advanced Reactor Fuels
- Improved Best Estimate Plus Uncertainty Methodology - Enhanced Validation & Benefits
- Predictive Maturity & Extrapolation
- FY11 Case Study Description
- Summary and Conclusion

FCRD – AFC Pursing A Science Based Approach To Advanced Fuels Development

- *Enhancing our fundamental understanding* of fuel and materials behavior under irradiation is critical
- Develop a *predictive capability* for simulating the phase and microstructural behavior of fuels and materials
- Integration of experiments, theory and modeling and simulation is *essential*



- M&S should help fuel qualification by
  - targeted testing for *a limited number* of fuel compositions
  - to quickly *interpolate (or extrapolate*, when possible) the empirical database to the entire range of variables

Regulatory Requirements for Fuel Qualification

- Provide assurance that
  - The fuel system is *not damaged* as a result of normal operation and Anticipated Operational Occurrences
  - Fuel system damage is *never so severe* as to prevent control rod insertion when it is required
  - The number of *fuel rod failures is not underestimated* for postulated accidents
  - Coolability is always *maintained*

- The analysis of reactor fuel is typically done with an analytic model that has been validated from an extensive data set
  - Approval of the *analytic model & analytic method*
  - Verifying that the licensee has shown that the analytic *model and method are applicable to its new fuel design* and all conditions and limitations are met

Use of Extensive of Modeling and Simulation

- The use of M&S tools as means of demonstrating that a design can meet NRC requirements is *not new* and has precedence
  - *CSAU (Code Scaling and Analysis of Uncertainty)* with the goal of demonstrating compliance with fuel cladding temperature criteria
  - Guidance on use of analytic or evaluation models
    - *Reg-Guide 1.157* (specific to fuel cladding, CSAU)
    - *Reg-Guide 1.203* (generic approach)

- *Need to be improved* to resolve new arising challenges
  - SMR workshop proposed *Performance-Based Framework*
    - Developing the *data and methods* to support a performance-based licensing frame
  - *An enhanced framework* for FRCD applications may be needed

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Challenges in Licensing Advanced Reactor Fuels

- **Schedule** will not allow up front determination of all data (developed *simultaneously* with code development and validation)
- **Data sufficiency** for validation to achieve licensing objectives? Requires a method "*Predictive Maturity*" & Method must *allow efficient feedback* to experimental design
- **Terminology** – *Complex chemical and physical process produce composition, properties* and conditions but must able to predict or estimate the effect of processes on properties
- **Identification of Phenomena** - Numerous chemical and physics processes occur at various length scales. A challenge is *how to do a PIRT* when the experience base does not exist or *developing parallel*?
- **Multi Scale Validation** - *Several different simulations at many scales* could occur simultaneously or in a serial fashion. *How multi-scale coupled validation* requirements and its process requirements should be addressed?
- **Review**
  - Focus of NRC Reg-Guides is ultimately showing compliance with a regulation
  - Challenge is *how to adapt the traditional BE+U method* to account for above issues
  - Development of a potential methodology will require early *NRC buy-in* and involvement

CSAU Overview: Evaluation Methodology

Element 1
Requirements and Code Capabilities

Scenario requirements, code capabilities, applicability, and limitations, identification of important phenomena

Element 2
Assessment and Ranging of Parameters

Code predictions against experimental data, and accuracy, scale-up capability, bounding calculations

Element 3
Sensitivity and Uncertainty Analysis

Simple and direct statement of the calculated uncertainty in the primary safety criteria, collect and combine individual contributors to uncertainty into the required 95% probability statements with biases

Improved Best Estimate Plus Uncertainty Methodology Including Advanced Validation Concepts to License Evolving Nuclear Reactors

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Element 1
Scope and Requirements

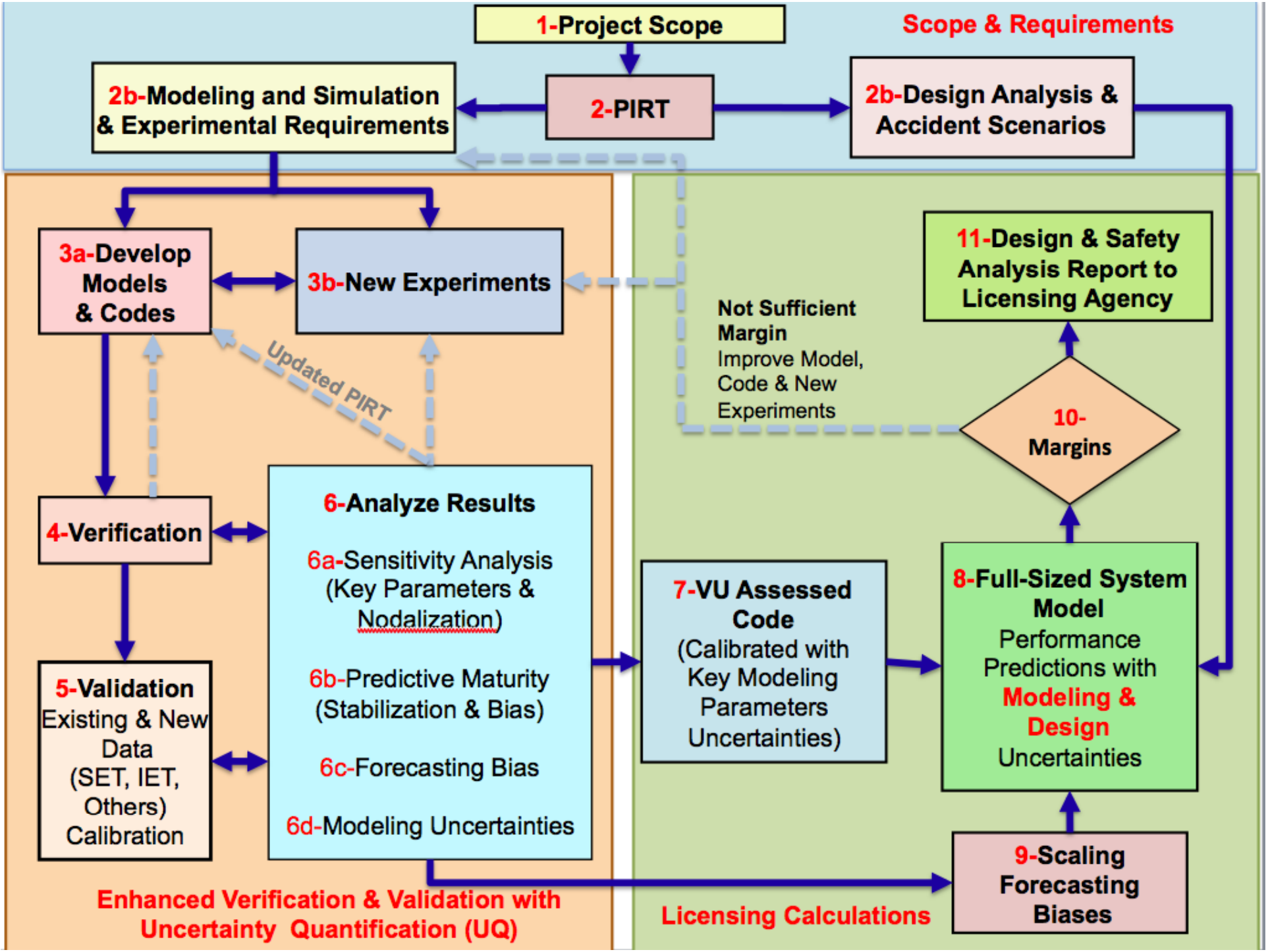
Scope of project, design analysis, accident scenarios, modeling and simulation and experimental requirements using identification of important phenomena methodology

Element 2
Enhanced Verification & Validation with Uncertainty Quantification

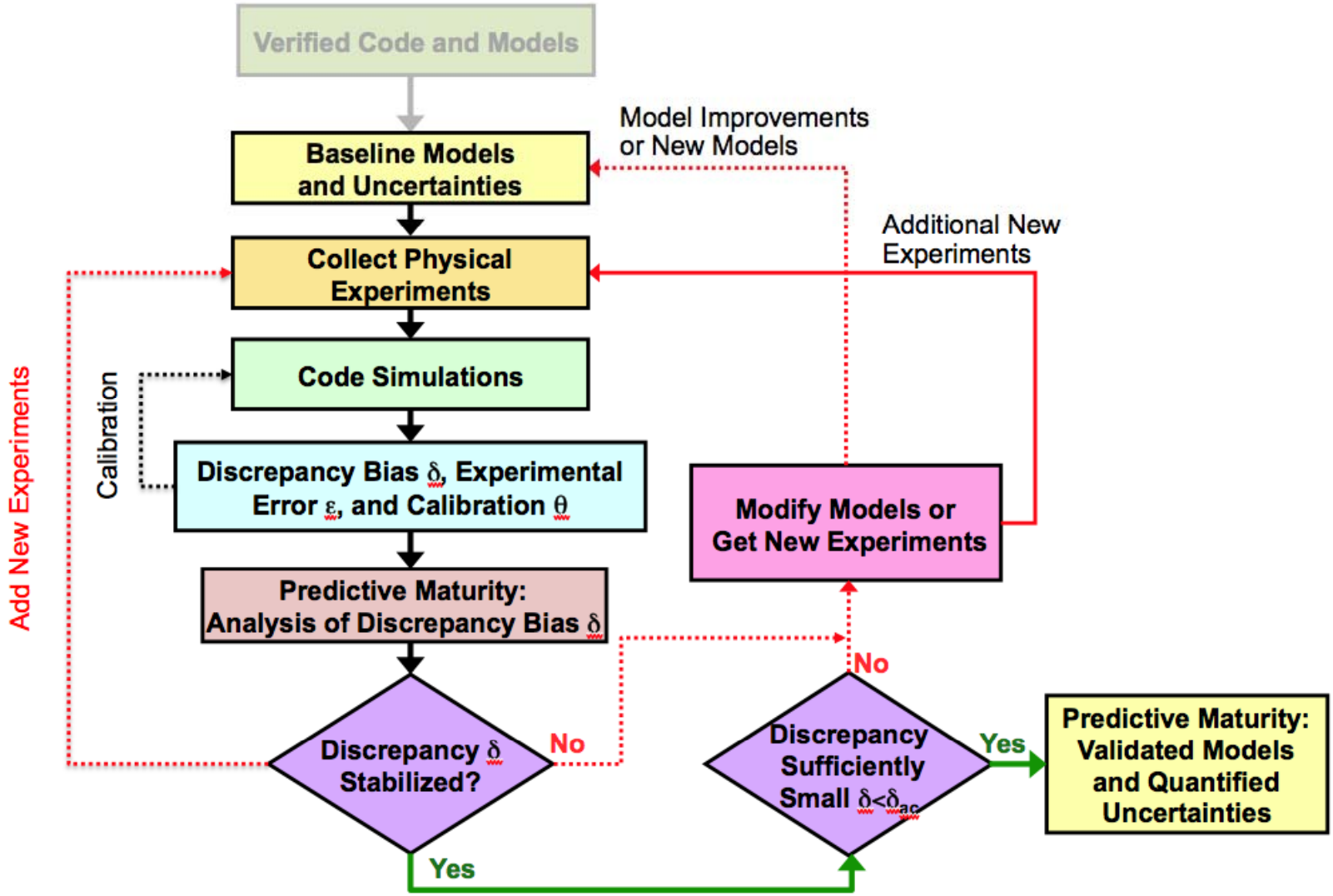
Development of models and codes, verification, enhanced validation and analysis (sensitivity, key model parameters, calibration, predictive maturity, modeling with uncertainty quantification), definition of new experiments & modeling needs (updated PIRT)

Element 3
Licensing Calculations

Full scale calculations with a VU assessed code using key modeling parameters and manufacturing uncertainties to drive a simple and direct statement of the calculated uncertainty in the primary safety criteria, collect and combine individual contributors including scaling and forecasting biases to uncertainty into the required 95% probability statements with biases


1-Project Scope
Scope & Requirements
2b-Modeling and Simulation & Experimental Requirements
2-PIRT
2b-Design Analysis & Accident Scenarios
3a-Develop Models & Codes
3b-New Experiments
Updated PIRT
Not Sufficient Margin
Improve Model, Code & New Experiments
11-Design & Safety Analysis Report to Licensing Agency
10-Margins
4-Verification
6-Analyze Results
6a-Sensitivity Analysis (Key Parameters & Nodalization)
6b-Predictive Maturity (Stabilization & Bias)
6c-Forecasting Bias
6d-Modeling Uncertainties
7-VU Assessed Code (Calibrated with Key Modeling Parameters Uncertainties)
8-Full-Sized System Model Performance Predictions with Modeling & Design Uncertainties
5-Validation Existing & New Data (SET, IET, Others) Calibration
9-Scaling Forecasting Biases
Enhanced Verification & Validation with Uncertainty Quantification (UQ)
Licensing Calculations

Enhanced Validation Aiming Minimizing Number of New Experiments By Proving Robust Predictive Capability



Improved Best Estimate Plus Uncertainty Methodology Extends Scope of Questions to be Addressed

Code Calculations Should Address Three Questions

- **CSAU**
  - Has the code the capability to *scale up phenomena* observed in small-scale test facilities to full-scale nuclear power plants?
  - Can the code be *applied to safety studies* of a particular scenario or a set of scenarios for a given plant design?
  - What is the *uncertainty with which the code calculates* important parameters, say the PCT in full-scale NPP?

- **Extended CSAU** (In addition to above questions)
  - Has the code the *predictive capability with quantified uncertainties* to the scale up phenomena in new or modified multi scale multi physics coupled advanced models developed in a *data sparse environment?*
  - Does the uncertainty in code calculated performance parameters include *all known potential uncertainty contributors* in every scale used in code calculations?

Improved Best Estimate Plus Uncertainty Methodology Extends Points To Consider

- **CSAU**
  - Effect of *scaling*
  - Effect of *tuned parameters* on NPP calcs
  - Scenarios producing nonconservative results due to *compensating errors*
  - Reasons for *disagreements* between data and calculations
  - *Effects of noding* and other adjusted numerical parameters
  - *Correlations not supported* by data and their effects

- **Extended CSAU** (in addition to above)
  - *Uncertainty in code calibration* parameters
  - *Predictive ability of the code* with respect to NPP calculations
  - *Stabilized calibration* & bias
  - *Guide designing new* experiments
  - *Forecasting uncertainty* in extrapolations

Enhanced Validation - Sensitivity Example from LIFE IV- Initial Results

	OUTPUT COLOR CODE			
Central Hole	Fission Gas Release	Axial Column Strain	Cladding Radial Strain	

Model Parameters	% Contribution to Uncertainty			
Fuel Creep 5	77.16%	26.60%	11.78%	3.54%
Cladding Temperature Axial Z1	48.44%	3.03%	1.48%	
Fission Gas Pore Migration 1	31.56%	12.89%	5.28%	
Fuel Creep 6	29.58%	24.85%	23.59%	4.18%
Fuel Creep 8	13.32%	12.27%	10.80%	2.44%
Fuel Thermal Conductivity 2	10.13%			
Oxygen:Metal Ratio	8.76%	5.90%	3.38%	2.09%
Smeared Density	7.42%	6.82%	3.10%	
Fission Gas Release 1	7.25%	1.57%		
Fission Gas Release Incubation 1	6.73%			
Fission Gas Release 2	4.88%			
Fuel Thermal Conductivity 2	4.51%	1.59%		
Pressure-Surface Tensions of Fission Gas Bubbles 2	3.60%	3.31%	2.32%	
Fuel Heat Capacity 2	3.26%			
Cladding Thermal Expansion 1	3.22%			
Fuel Heat Capacity 3	2.66%			
Fuel Thermal Conductivity Burn Up	2.02%			
Cladding Specific Heat 2	1.94%			
Fuel Thermal Conductivity 3	1.86%	1.71%		
Fuel Creep 7	1.83%			
Peak Power	1.74%			
Fission Gas Release in Columnar Zone	1.61%			
Fuel Surface Roughness	1.59%			
Reduce Fission Pore Velocity at Low Burn Up	1.57%			
Fuel Poisson Ratio	1.49%			

Initial Findings – 69 Paramaters

- Fuel Creep
- Fission Gas
- Fuel conductivity
- O/M, Clad Thermal Expansion
- Fuel Heat Capacity
- Will be repeated after calibration for investment decision
- Need to consider with all calibration data

Proposed Quantitative Maturity Metric Considering Attributes of *Coverage, Discrepancy, Complexity*

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Predictive Maturity Index (PMI)

- *PMI ~ f(η_C, N_K δ_S)*
- *0 ≤ PMI ≤ 1,*
- PMI = 0 ~ *no maturity*
- PMI = 1 ~ *perfect maturity*
- "0" and "1" are *asymptotic limits*

- Four properties and asymptotic behavior of a monotonic function

$$\frac{\partial \mathrm{PMI}}{\partial \eta_C} \geq 0 \qquad \lim_{\eta_C \to 0} \mathrm{PMI} = 0$$

$$\frac{\partial \mathrm{PMI}}{\partial \delta_S} < 0 \qquad \lim_{\delta_S \to 1} \mathrm{PMI} = 0$$

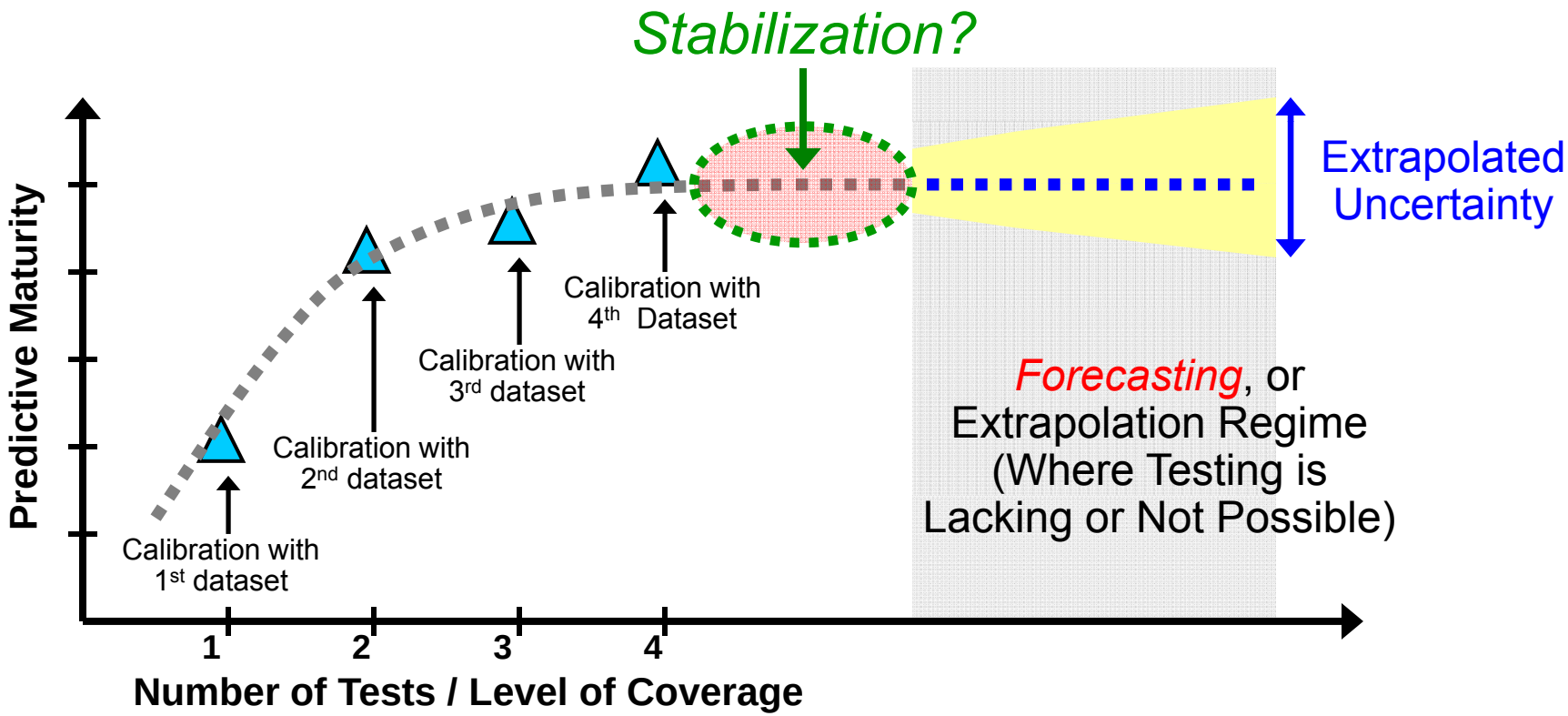
$$\frac{\partial \mathrm{PMI}}{\partial N_K} \leq 0 \qquad \lim_{N_K \to \infty} \mathrm{PMI} = 0$$

$$\lim_{\delta_S \to 0,\ \eta_C \to 1} \mathrm{PMI} = 1$$

$$\mathrm{PMI} = \mathrm{F}(\eta_C; N_K; \delta_S) = \mathrm{PMI} = \eta_C \times \left(\frac{N_R}{N_K}\right)^{\gamma_1} \times (1-\delta_S)^{\gamma_2} \times e^{(1-\eta_C^2)^{\gamma_3} - \delta_S^2}$$

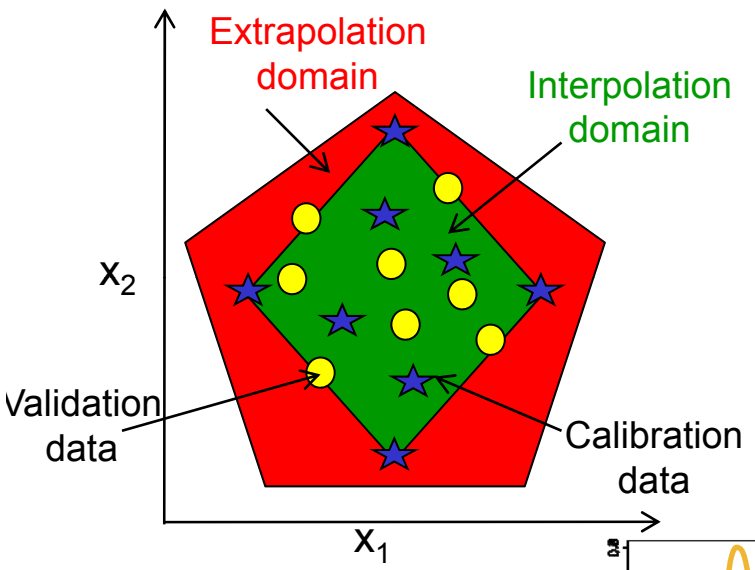
Code Calibrations Should Reach Stabilized Stage

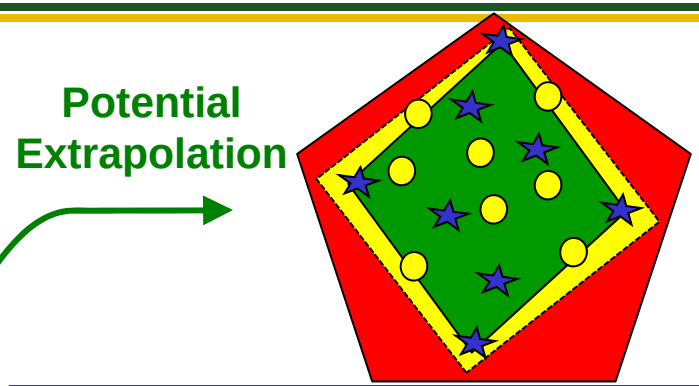
- *As more datasets are used, does predictive maturity reach a stable asymptote?*

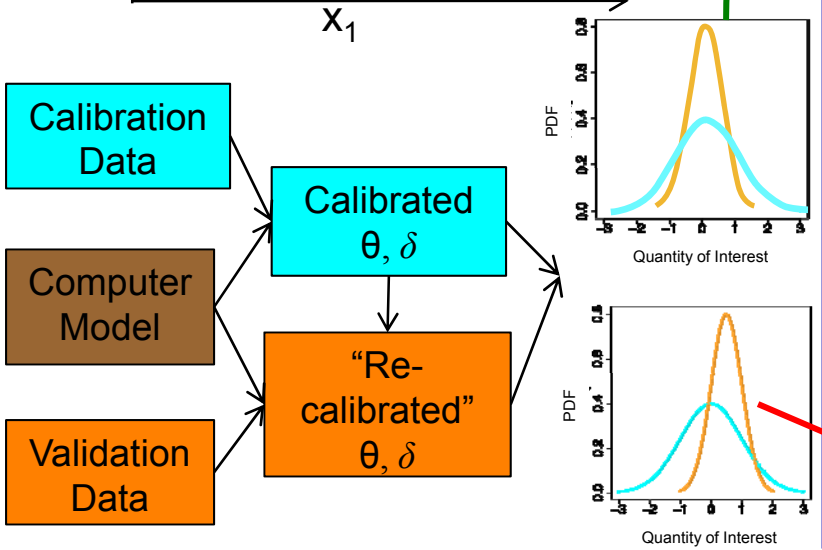


- Stabilization is necessary for *forecasting* (extrapolation)

Potential Extrapolation Requirements







- **Potential Extrapolation**
  - –Posteriors of calibration & validation data *similar*
  - –if δ model *is believed* in extrapolation domain (δ ~zero or physics-based at level of hierarchy requiring extrapolation)
  - –Empirical δ models can only be extrapolated with great care; quantitative guidelines needed
  - –Statistical criteria & design and physics guidance need to be developed to define potential region of extrapolation
- **No Extrapolation** ~ Recalibrated posteriors of calibration & validation data *significantly differs*

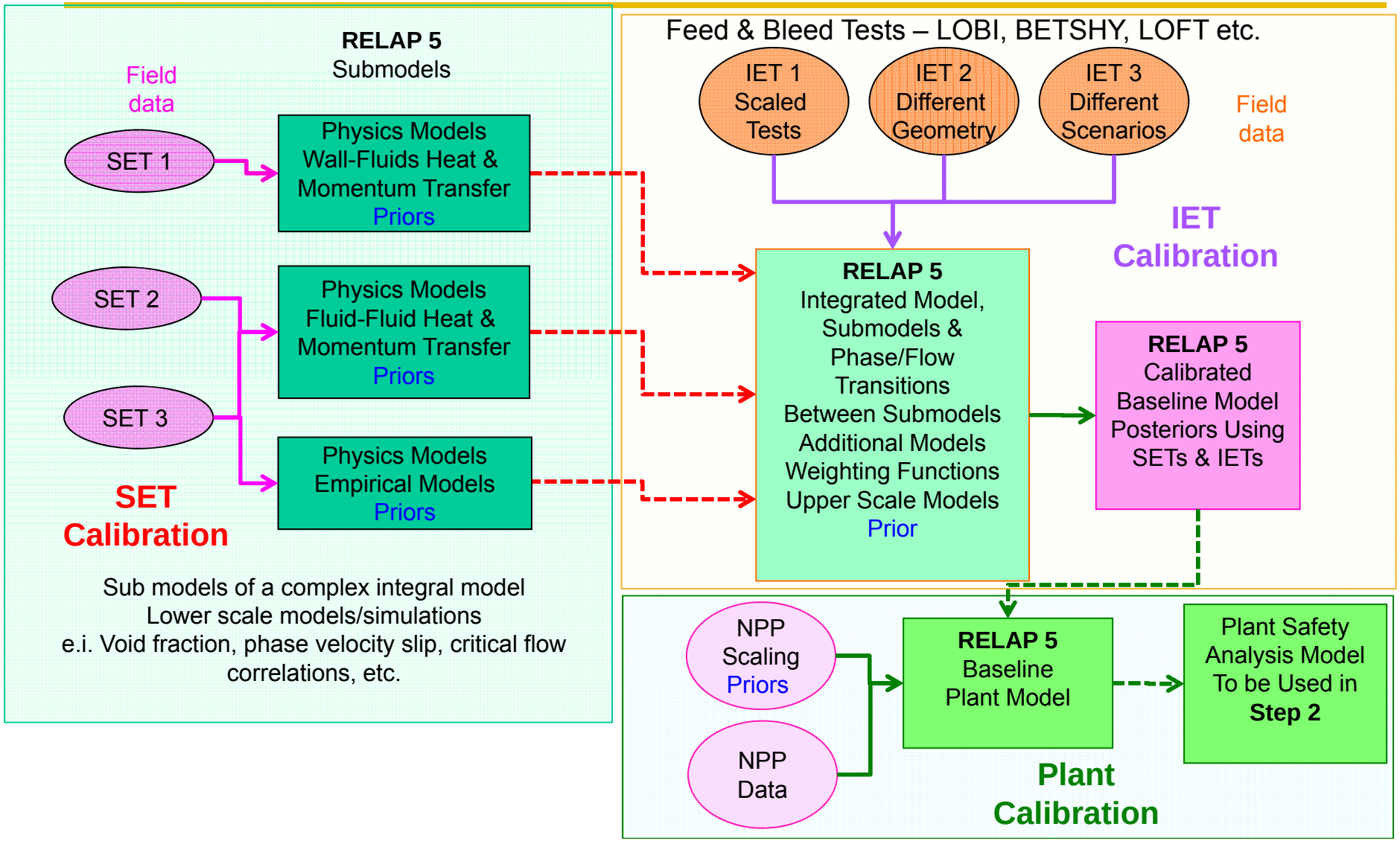
Case Study – Experiment Design and Optimization for Scenario Assessment for Feed and Bleed Analysis

- ***Feed and Bleed Cooling in PWRs***
  - Reactor core cooling is maintained by injection coolant with pumped emergency core cooling systems and removing the heated/vaporized fluid via pressurizes power operated relief valve(s) (PORV(s))
  - Loss of secondary heat sink, reactor has scrammed, power operated relief valve(s) are operative, pressurizer heaters are off, primary recirculation pumps are tripped
  - Simple mass and energy balance bounding analysis has uncertainties due to two-phase flow through PORV, actual heat load, the operating range of the HPI system and transient behavior
  - Safety basis is based on calculations by RELAP/TRAC modeling and scaled integral effect testing

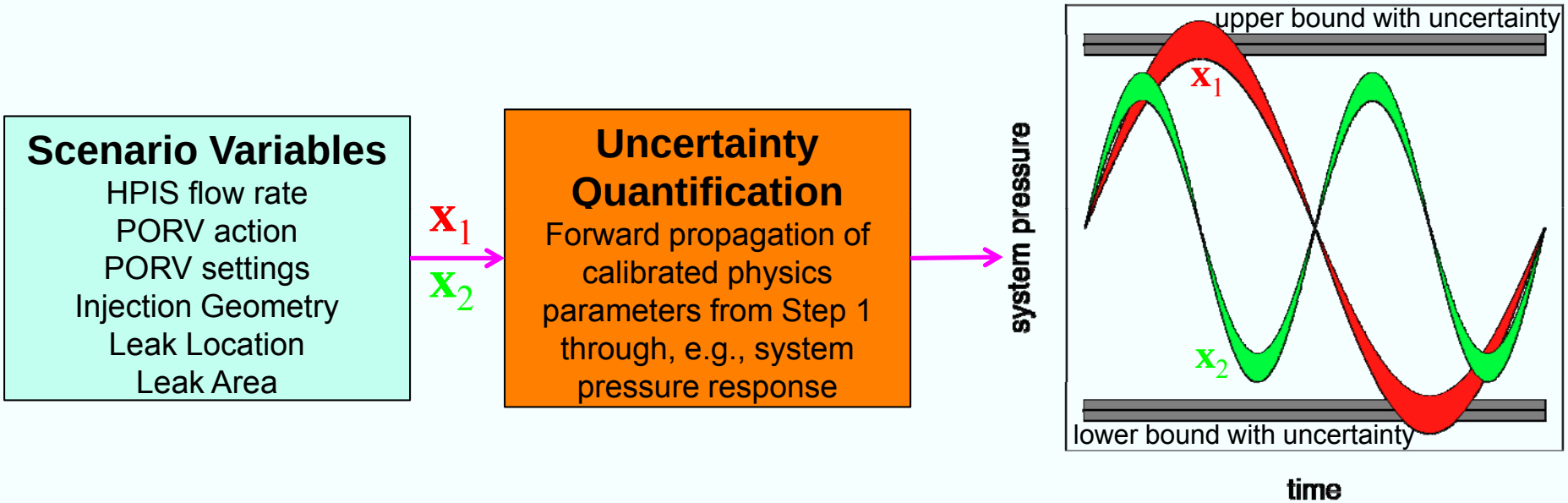
- Concerns on potential scenarios resulting in unsustainable operations due to undefined combination of PORV actions and settings, injection geometry and locations, leak sizes and locations

- ***Case Study*** - Apply this methodology to reduce/eliminate the uncertainty in undetected scenarios

Case Study- Step 1- Simultaneous Calibration & Uncertainty Propagation Scheme Using IET data



Case Study Step 2



- Identify regions of scenario space leading to violation(s) of bounds on system response variables
- Resource allocation (new experiments) to reduce physics uncertainty under certain scenarios (e.g. x_1) or region(s) of scenario space

Summary and Conclusion -

Now, It is a Good Time to Resume the National Working Group to Finalize the Development of the Extended Best Estimate + Uncertainty Methodology

- Traditional approaches to quickly develop and qualify advance fuels is *very challenging* without extensive use of M&S
- M&S has additional challenges to be addressed
- We propose using an extension of existing methods and guidance to *extend the "Best Estimate + Uncertainty"* to address these challenges
- New methodology suggests a formalism *(predictive maturity)* to *quantify an adequate level of validation* with respect to existing data so that required testing can be *minimized for cost saving* purposes
- Case study will demonstrated the value
- Methodology is *at conceptual level, needs to be debated* by stakeholders
- We propose to form/resume *a national working group* to finalize the development of the extended best estimate plus uncertainty methodology as a licensing option for new NE technologies

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Additional Slides

Enhanced Validation- Sensitivity Example from LIFE IV

- What is different in our method
  - Multi *parameter-to-parameter* interaction consideration
  - *High number* of model parameters
  - New *screening* method
- *69 input parameters* varied : design, operating, and materials properties parameters (orange) and calibration parameters (yellow

Fuel Heat Capacity 1	FFHC1	Oxygen:Metal Ratio	OMR
Fuel Heat Capacity 2	FFHC2	Pu Weight Fraction	PUWF
Fuel Heat Capacity 3	FFHC3	Peak Power	PP
Fuel Heat of Fusion	FHF	Cladding Temperature, Axial Zone 1	CT1
Fuel Thermal Expansion 1	FTE1	Cladding Temperature, Axial Zone 1	CT2
Fuel Thermal Expansion 2	FTE2	Cladding Temperature, Axial Zone 1	CT3
Fuel Hot Pressing and Densification 1	FHPD1	Cladding Temperature, Axial Zone 1	CT4
Fuel Hot Pressing and Densification 2	FHPD2	Cladding Temperature, Axial Zone 1	CT5
Fuel Hot Pressing and Densification 3	FHPD3	Cladding Roughness	CR
Fuel Hot Pressing and Densification 4	FHPD4	Fuel Surface Roughness	FR
Fuel Creep 4	FFC4	Thermal Conductivity 1	TC1
Fuel Creep 5	FFC5	Thermal Conductivity 2	TC2
Fuel Creep 6	FFC6	Thermal Conductivity 3	TC3
Fuel Creep 7	FFC7	Helium Accomadation Coefficient (conductivity)	HAC
Fuel Creep 8	FFC8	Fission Gas Release 1	FGR1
Fuel Shear Modulus 1	FSM1	Fission Gas Release 2	FGR2
Fuel Shear Modulus 2	FSM2	Pressure due to surface tension of fission gas bubbles 1	PGI1
Fuel Shear Modulus 3	FSM3	Pressure due to surface tension of fission gas bubbles 2	PGI2
Fuel Shear Modulus 4	FSM4	Fuel Swelling Rate Constant at low burn up	FSRC
Fuel Shear Modulus 5	FSM5	Fission Gas Release Incubation 1	FGRI1
Fuel Poisson's Ratio	FPR1	Fission Gas Release Incubation 2	FGRI2
Cladding Thermal Expansion 1	CTE1	Fission Gas Pore Migration 1	FGPM1
Cladding Thermal Expansion 2	CTE2	Fission Gas Pore Migration 2	FGPM2
Cladding Specific Heat 1	CSH1	Equiaxed Zone Radius Criterion	EZRC
Cladding Specific Heat 2	CSH2	Columnar Zone Radius Criterion	CZRC
Cladding Thermal Conductivity 1	CTC1	Fuel Thermal Conductivity as a function of Burn Up 1	FTCBU1
Cladding Thermal Conductivity 2	CTC2	Fuel Thermal Conductivity as a function of Burn Up 2	FTCBU2
Cladding Shear Modulus 1	CSM1	Fission Gas Swelling Rate Constant	FGSRC
Cladding Shear Modulus 2	CSM2	Gap Closure Rate Constant	GCRC
Cladding Poisson's Ratio 1	CPR1	Reduce Fission Pore Velocity at low burn up	RFPV
Cladding Poisson's Ratio 2	CPR2	Fission Gas Release in Columnar zone	FGRCR
Cladding Corrosion by Sodium 1	CIC1	Axial Vapor Phase Transport Rate Constant	AVPTRC
Cladding Corrosion by Sodium 2	CIC2	Crack Elasticity	CE
Fuel Density	FD	FCMI to Yield	FCMIY
Smeared Density	SD		

- Data from 5 pins for mechanical, thermal calibration including high burn up data

Prediction Discrepancy – Epistemic Uncertainty

- Predictive maturity also depends on the extent to which predictions of the model match the physical test data
- We start by postulating a model of prediction accuracy

Measurements — Predictions — Discrepancy

$$\overbrace{y^{Test}}^{\text{Measurements}} = \overbrace{y(p;\theta)}^{\text{Predictions}} + \overbrace{\delta(p)}^{\text{Discrepancy}} + \varepsilon^{Test}$$

Control Parameters (p)

Calibration Variables (θ)

$$\delta_S = \frac{\|\delta(p)\|}{\|y(p;\theta)\|}$$

- Our metric of prediction accuracy is a *discrepancy* term that captures residual differences between predictions and measurements that cannot be compensated for by adjusting the calibration variables (θ)

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Challenges - Terminology

Chemical Processes

Phase transformations
Phase stability
Oxidation/Reduction
Corrosion
Non-stoichiometry
Species formation

Physics Processes

Neutronics/Kinetics
Fission product generation, release, diffusion & accumulation
Vacancy/Interstitial movement
Oxidation
Deposition
Transport/Migration
Diffusion
Aggregation
Conduction
Convection
Radiation
Swelling
Gas generation
Creep
Melting
Restructuring
Interactions (FCMI, FCCI)
Annealing
Cracking (separation)
Precipitation
Hardening/Embrittlement

Composition

Cracks
Radiation Defects
vacency interstitual
dislocations
small clusters
voids (central void)
Grain features
Boundaries (grain, material)
Metallic inclusion
Fission gas
Porosity

Properties

Thermal conductivity
Melting temperature
Heat capacity
Enthalpy
Thermal expansion
Diffusivity
Specific heat
Porosity
Heterogenity
Anisotropy
Burn-up
Solubility
Elasticity

Conditions*

Pressure
Temperature
Burn-up

Note: Chemical and Physics Processes produce Composition, Properties and Conditions but must be able to predict or estimate the effect of processes on properties.

* Physical state at a given time

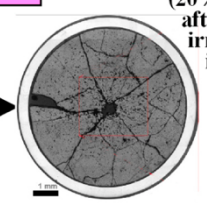
Engineering Scale Processes (Stan)

Neutronics (fission and neutron diffusion)
Heat transfer (conduction, convection, radiation)
Mass transport (species diffusion and gas accumulation)
Thermo-mechanics (deformation, such as swelling)
Fluid flow (to model the coolant, if necessary)

Start

Unirradiated Fuel

Changes with Time Under Irradiation Conditions



AM-1 Test (20% Pu-Mox) after 10 min irradiation in Joyo

Key Fuel Performance Modeling & Simulation Capabilities

Fuel element temperature distribution
Stress-strain state, fuel & cladding dimensions and FCMI
Irradiation effects (degradation, irradiation-induced creep, thermal creep, swelling, hardening, and embrittlement
Cladding wastage due to fuel-cladding chemical and coolant-cladding chemical interaction
Cladding failure
Heat transport from the clad into the coolant for all operating and design-base accidents

CSAU Overview: 14 Specific Steps In CSAU

Steps	Description
1	Specify scenario
2	Select NPP
3	Phenomenon identification and ranking table (PIRT)
4	Select frozen code
5	Provide code documentation
6	Step 6: Determine code applicability
7	Establish assessment matrix
8	Define nodalization for NPP
9	Determine code and experimental accuracy
10	Determine scaling effects
11	Determine effect of reactor input parameters and state
12	Performa NPP sensitivity calculations
13	Combine biases and uncertainties
14	Total uncertainty to calculate specific scenario in a specific NPP

Feed and Bleed Integral Test

- LOBI BT-02 - loss of main and aux feed water with PORVs opened, HPSI
- LOBI BT-17 – loss of main and aux feed water with secondary side feed and bleed, LPSI
- BETHSY 5.2e – loss of feedwater with HPSI and LPSI , and SITs
- BETHSY 5.2c2 – primary feed and bleed (high pressure) total loss of feed water
- SPES SP-ST-01 – station blackout, bleed and feed, accumulator injection…core uncovery
- PKL III B1.2 – loss of feedwater with sec feed and bleed, no injection available
- UPTF, TRAM B2 – high pressure primary side feed and bleed via pressurizer SEMISCALE PL-3E – station blackout feed and bleed recovery
- BETHSY 6.5 – pressurizer top break
- LSTF SP-PR-02 – pressurizer top break, 0.5%, wo HPI, no AFW
- MIST 330100 – PORV lift, feed and bleed experiment
- LOFT FW-1 – loss of feed water primary feed and bleed
- LSTF- TR-LF-06 – TMLB' with pump seal leak, primary F&B
- LSTF TR-LF-07 – total loss of feed water, primary F&B
- LSTF SB-HL-05,06 – 0.5% HL break, wo HPSI, primary F&B
- LSTF SB-CL-22 – 5% CL break, wo HPSI, secondary F&B
- LSTF SB-CL-25 – 0.5% CL break, recovery with secondary ARV

Other tests to validate SBLOCA capability

- SEMISCALE – S-07-10D (NUREG/CR-1641, EGG-2065, Dec 1981), and (EGG-SEMI-5021 July 1980), S-07-10, S-UT-8(EGG-SEMI-5827, mar 1982), S-LH-1, S-02-6
- ROSA-IV SB-CL-01
- LOFT L3-5, L3-5A, L3-6,L8-1
- See NUREG/CR-4945 (EGG-2509,July 1987) for integral testing

Level swell

- Oak Ridge THTF 3.09-10I, J,K,L,M,N,AA,BB,CC,DD,EE,FF (see NUREG/CR-2456)
- Westinghouse 336 Rod Bundle Uncovery Tests (EPRI NP-1692, Vol 1, 1981) Test 718
- GE Level Swell Tests (EPRI NP-1527, Oct 1981).
- BNWL-1411, June 1970 'Experimental High Enthalpy Water Blowdown From a Simple Vessel Through a Bottom Outlet '
- BNWL-1463, Feb 1971 "Coolant Blowdown Studies of a Reactor Simulator Vessel Containing a Perforated Sieve Plate Separator"

Improved Best Estimate Plus Uncertainty Methodology - Steps

	CSAU		Improved CSAU
Steps	**Description**	**Steps**	**Description**
1	Specify scenario	1	Scope of Project
2	Select NPP	2	Phenomenon Identification and Ranking Tables
3	Phenomenon identification and ranking table (PIRT)	3	Modeling and Simulation and New Experimental Requirements
4	Select frozen code	4	Verification
5	Provide code documentation	5	Validation
6	Step 6: Determine code applicability	6	Analysis During Validation
7	Establish assessment matrix	6a	Sensitivity Analysis, Key Modeling Parameters, Nodalization
8	Define nodalization for NPP	6b	Predictive Maturity, Stabilization and Bias
9	Determine code and experimental accuracy	6c	Forecasting Bias
10	Determine scaling effects	6d	Modeling Uncertainties
11	Determine effect of reactor input parameters and state	7	VU-Assessed Code
12	Performa NPP sensitivity calculations	8	Full System Model and Predictions with Uncertainties
13	Combine biases and uncertainties	9	Step 9: Scaling and Forecasting Biases
14	Total uncertainty to calculate specific scenario in a specific NPP	10	Margins
		11	Design and Safety Analysis Report