Reactor Physics Nuclear Data Needs

presented to WANDA 2020 Workshop

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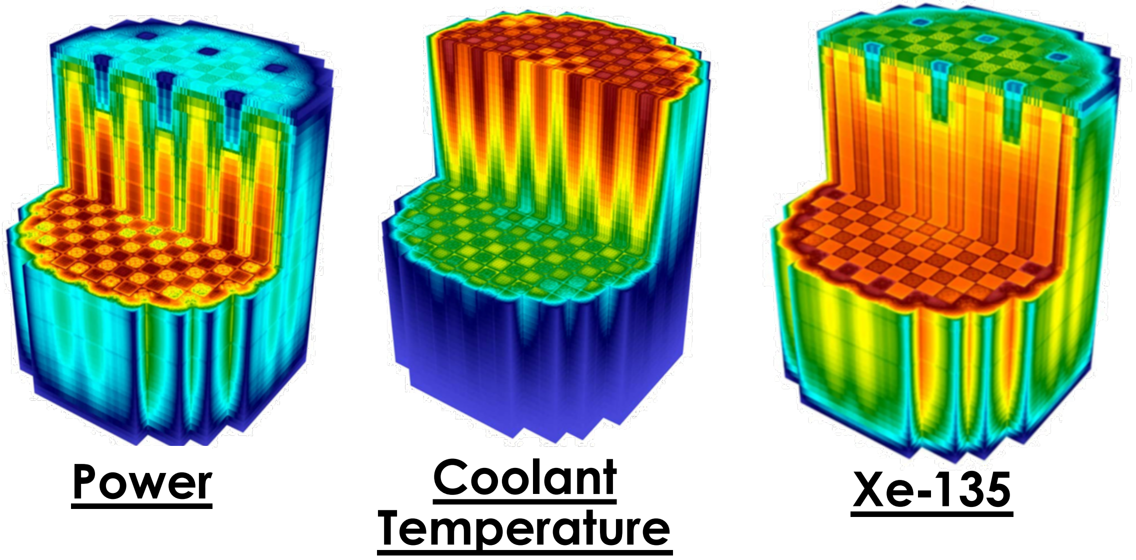
My Background

- **2009** NC State Neutron transport methods Ph.D.
  - interned at BNL, INL, LANL
- **2009-2012** at Swiss National Lab doing reactor safety analysis for Beznau units 1&2
- **2012-2017** at ORNL as SCALE developer/analyst/trainer
  - co-designed Polaris lattice physics for NRC
  - co-developed Sampler uncertainty quantification platform
  - lead modernization of ORIGEN depletion/decay code for DOE
    - ANL and INL collaborations
  - analysis work focusing on severe accidents for LWRs with SNL, uncertainty quantification
- **2017-current**
  - Multiphysics team lead within Reactor Physics group (CASL VERA developers)
  - SCALE deputy manager then director



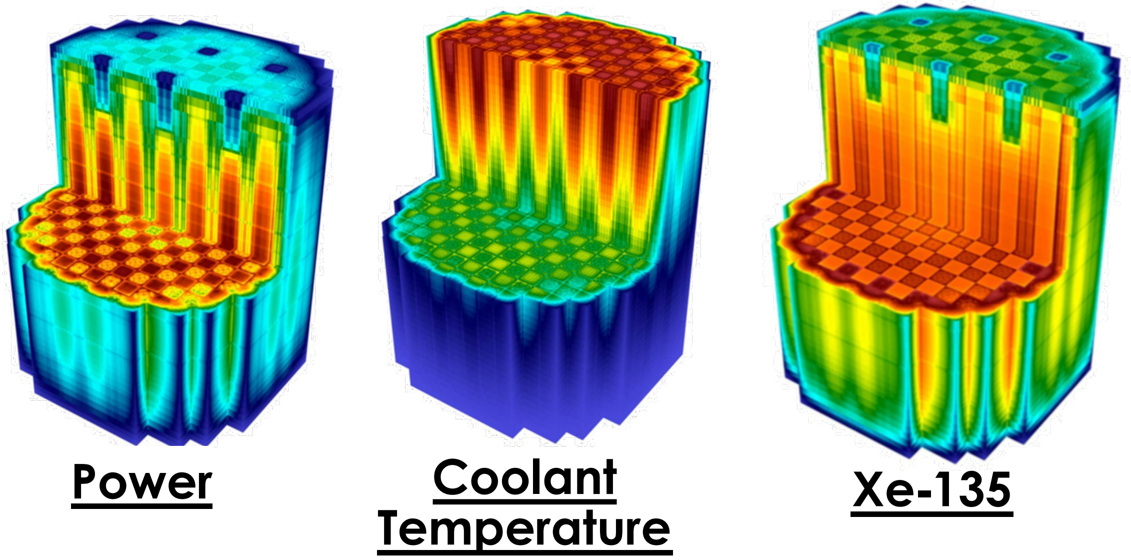
DOE CASL core simulator (VERA)
Watt's Bar Unit 2 Blind Predictions of Startup

Table 4-2. Control Bank Worth Results

Control Bank	Measured (pcm)	Original Prediction (pcm)	Latest MPACT (pcm)	Shift (pcm)	Original Prediction Error	Latest VERA Error	Shift Error
Bank D	1304	1320	1311	1322	1.2%	0.5%	1.4%
Bank C	1061	1078	1065	1076	1.6%	0.4%	1.4%
Bank B	794	821	815	816	3.4%	2.6%	2.7%
Bank A	910	912	904	913	0.2%	-0.6%	0.3%
Bank SD	438	452	451	449	3.3%	3.0%	2.6%
Bank SC	447	452	450	450	1.0%	0.7%	0.6%
Bank SB	1056	1072	1063	1070	1.5%	0.7%	1.4%
Bank SA	424	420	420	415	-1.0%	-1.1%	-2.1%
Total	**6435**	**6526**	**6478**	**6512**	**1.4%**	**0.7%**	**1.2%**
St. Dev.					**1.4%**	**1.4%**	**1.5%**

What do Reactor Physics Codes Calculate?

– **Nuclide distributions** (delayed neutron precursors, actinides, and fission products that drive evolution of system)
– **Energy/power distributions** (nominal power distribution, shutdown decay heat)
– **Reactivity** (shutdown margins, control bank worths)
– **Temperature and density** (assess limits, thermal feedback)



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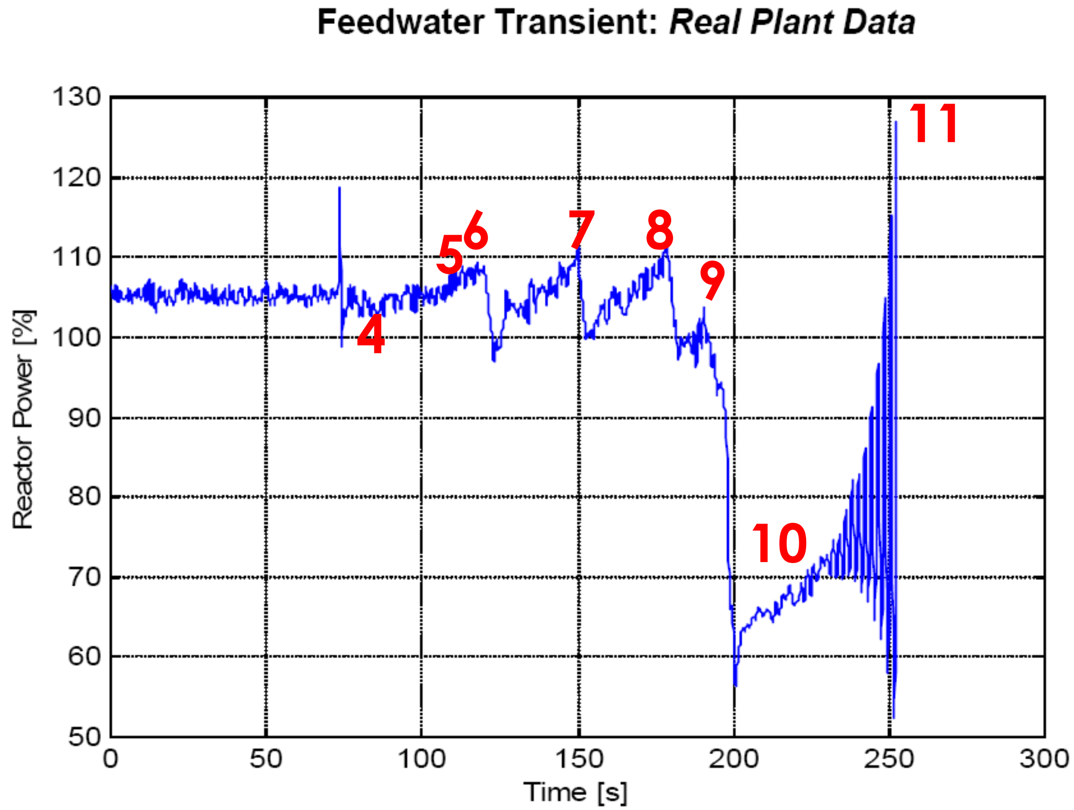
Reactor Physics Codes typically have two "modes"

- **Kinetics**
  - **what**: solve coupled neutron transport and delayed neutron precursor equations with T/H feedback
  - **why**: understand safety limits, accident scenarios, and power maneuvers (seconds/hours timescale)
- **Depletion**
  - **what**: solve coupled neutron transport and fuel depletion with total system power given and nominal density/temperature
  - **why**: understand operational limits (e.g. shutdown margins/reactivity coefficients at BOC/MOC/EOC), generate isotopics/decay heat for severe accident analysis or back-end transport/storage analysis (days/years timescale)

Oskarshamn-2 1999 BWR Stability Event



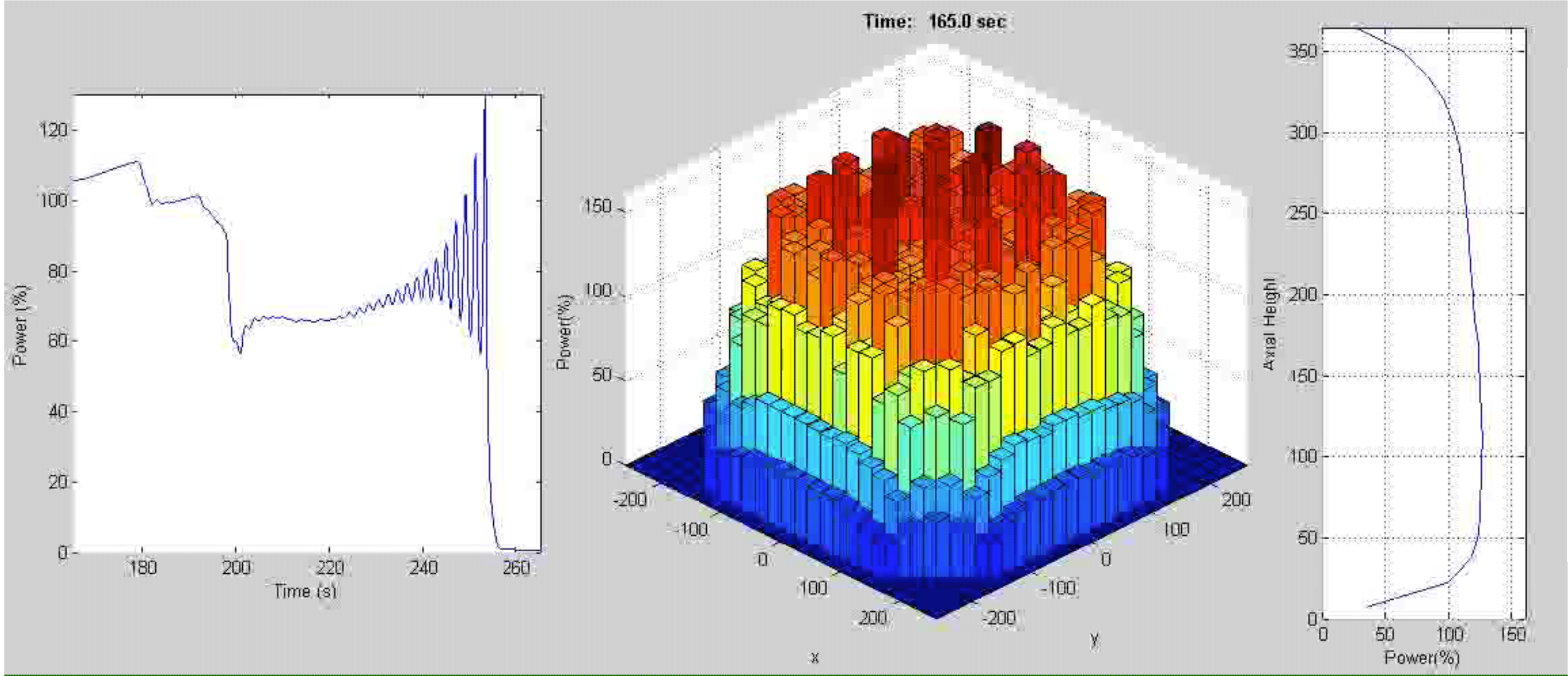
4. Loss of FW pre-heaters, FW flow remained constant.
5. Increased temp/lower density causes reactivity increase.

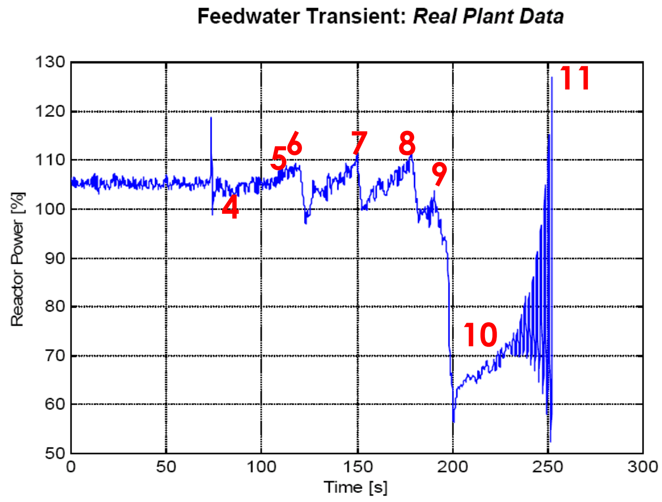
…

10. Eventually hit low flow/low power instability
11. Reactor trips

SCALE/TRITON+PARCS NRC Core Simulator

Oskarshamn-2 1999 BWR Stability Event: Kinetics simulation with total, radial, axial power





1. Short loss of external power.
2. Closure of turbine control valves and opening of the dump valves.
3. Generator power reduced, but no pump run-down – reactor remains at full power.
4. Loss of FW pre-heaters, FW flow remained constant.
5. Reduced FW temperature causes decrease in coolant temperature which causes power increase.
6. Recirc pump. run-down tripped on high power.
7. Continuing decrease of FW and coolant temperature causes power increase and trips recirc. pump run-down.
8. Continuing decrease of FW and coolant temperature causes power increase and trips recirc. pump run-down.
9. Operators trigger partial scram, recirc. pump run-down to minimum pump speed.
10. Continuing decrease of FW and coolant temperature pushes reactor into unstable conditions.
11. Reactor trips on high power signal.

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Nuclear Data used by SCALE Reactor Physics Codes

ENDF/B
Physics data
Thermal scattering law,
resonance data,
energy distributions,
fission yields, decay constants,
decay energy

Activation (JEFF)
Isomeric cross sections, activation reactions

Kinetics
nuclide-specific beta, neutron precursor data

Energy Release
nuclide-specific energy per capture/fission

Mass (NIST)
natural abundance, atomic mass

ENDF/B

- Used to calculate neutron/photon distributions, fission product generation rates, decay physics, shutdown
- ENDF/B VII.1 has overall good agreement with validation data *(critical benchmarks, spent fuel isotopics, decay heat measurements, in-core/ex-core reactor detector signals, boron letdown)*
- Propagating uncertainties seems to overestimate measurement bias uncertainty
- Fix-ups applied to deployed SCALE data
  - Move intermediate fission product yield energy from 0.5 MeV→2 MeV to be more consistent with how we calculate average energy of fission (Gauld)
  - Fission yield/decay consistency (Pigni)
  - Metastable id consistency, e.g. should m1 be lowest energy or longest half-life (Wiarda)

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Activation Data (JEFF/3.1-A)

- Used to calculate isomeric transitions, e.g. Am-241+n → g+Am-242m(12%), Am-242 (88%)
- No uncertainty/correlation available
- Still does not have some reactions, e.g. isotope production Th229 needed additional Ra,Ac isotopes from TENDL so now have 3rd xs library involved
- Fix-ups applied to deployed SCALE data
  - Ensure consistency on ENDF/B nuclides and JEFF nuclides
  - If ENDF/B xs is available, make sure isomeric transitions sum to ENDF/B value

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Kinetics Data (various sources)

- 6 delayed neutron groups with 2-energy group, actinide-dependent beta, lambda values hard-coded for ~10 actinides
- No uncertainty/correlation available
  - Should be correlated to chi-delayed, chi-bar?
  - Using existing cross section/decay uncertainty led to large ~15% beta-eff 1-sigma unc. with depletion
- Likely inconsistency with high-fidelity simulation of delayed neutron precursors, e.g.
  - We can explicitly simulate 1400 fission products from fission of 30 actinides
  - We know all the decay data that produces neutrons (e.g. β-n, spont. fiss.) and emission energy spectrum
  - Is this consistent with each actinide's chi-delayed?

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Energy Release Data (various sources)

- System-power level is a known/constraint in most depletion calculations
  - This "kappa" data turns relative/unnormalized reaction rates into absolute/normalized ones
  - Affects time evolution only
  - Capture energy in non-fuel is important too (stainless steel cladding and gadolinia absorber n,gamma)
- 1% change in important "kappa" ⇔ 1% change in definition of "burnup" among different codes/measurements
  Recent assumption of 5 MeV/capture Gd-155 instead of more accurate ~8 MeV/capture leads to noticeable few percent bias in low-burnup/high gadolinia fuel.
- No uncertainty/correlation available
  - Should be correlated to fission/capture xs?

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Mass/Abundance Data (NIST)

- Very convenient in many instances to specify material
  - density in g/cc
  - compositions in wt%
  - natural elements, e.g. iron
- NIST provides consistent source of up-to-date atomic masses and natural abundances
- Fix-ups applied to deployed SCALE data
  - SCALE/AMPX must process ENDF/B with evaluation mass for consistency with evaluation → then replace with NIST mass for consistency with SCALE composition processing
  - consistent nuclide ids for NIST element->isotope breakdowns
  - tricky cases like natural Tantalum with Ta180 (99.988%) and Ta180m (0.012%)

Recommendations from Reactor Physics

ENDF/B
Physics data
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- **Focus on ENDF/B completeness first**
  - Strive to be a comprehensive one-stop shop
  - SCALE would replace JEFF with ENDF/B activation
    FOA: *Model Oriented Nuclear Data Library (MONDL)*
  - Kinetics data is extremely relevant for advanced reactors
    High-priority?
  - Energy release data is almost always a source of inconsistency--our data differs by that used in reactor neutrino simulations by 10%
  - Pre-release testing (i.e. ADVANCE) includes some reactor physics validation cases
- Incorporate downstream fix-ups
  - yield/decay consistency within an ENDF/B version
  - identifier consistency across versions (e.g. metastable)
  - fission yield energy values (0.5 MeV->2 MeV) and recommended RP usage
- Ensure data formats (GNSD) should have uncertainty for every value and potential for correlation between any two values

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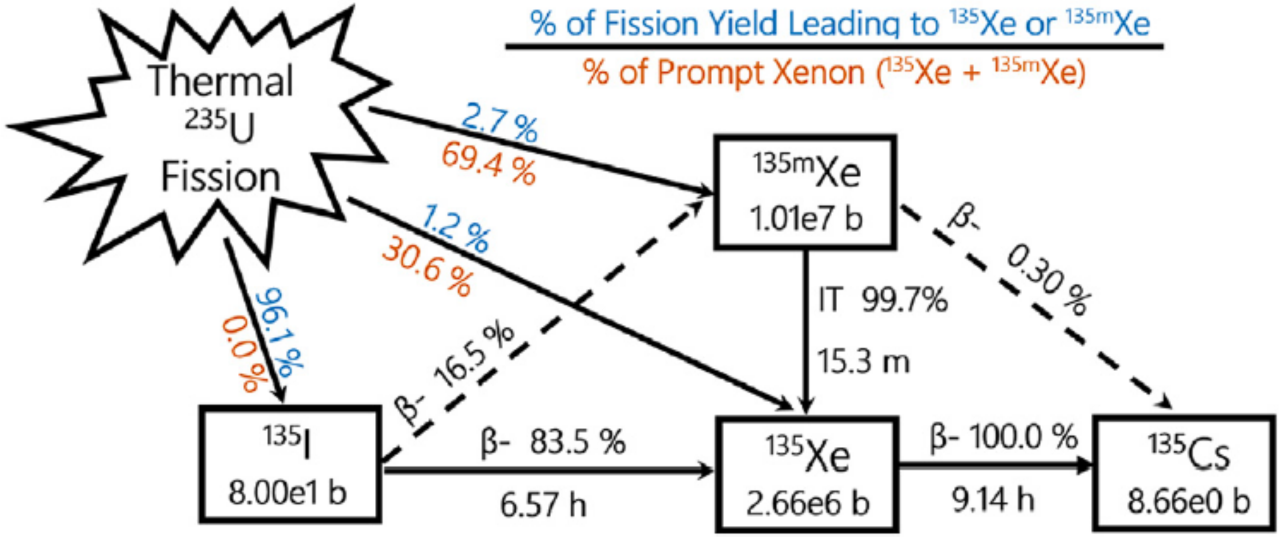
Questions?

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy and by the US Nuclear Regulatory Commission (NRC); the presentation of the work is sponsored by the NRC.

Missing Data: Xe-135m

- ENDF/B and backup Activation (JEFF) does not have Xe-135m cross section
- ENDF/B has decay data
- When developing CASL 300 nuclide depletion chain
  - Redirect all decay of I-135 to Xe-135?
  - Include Xe-135m in chain?



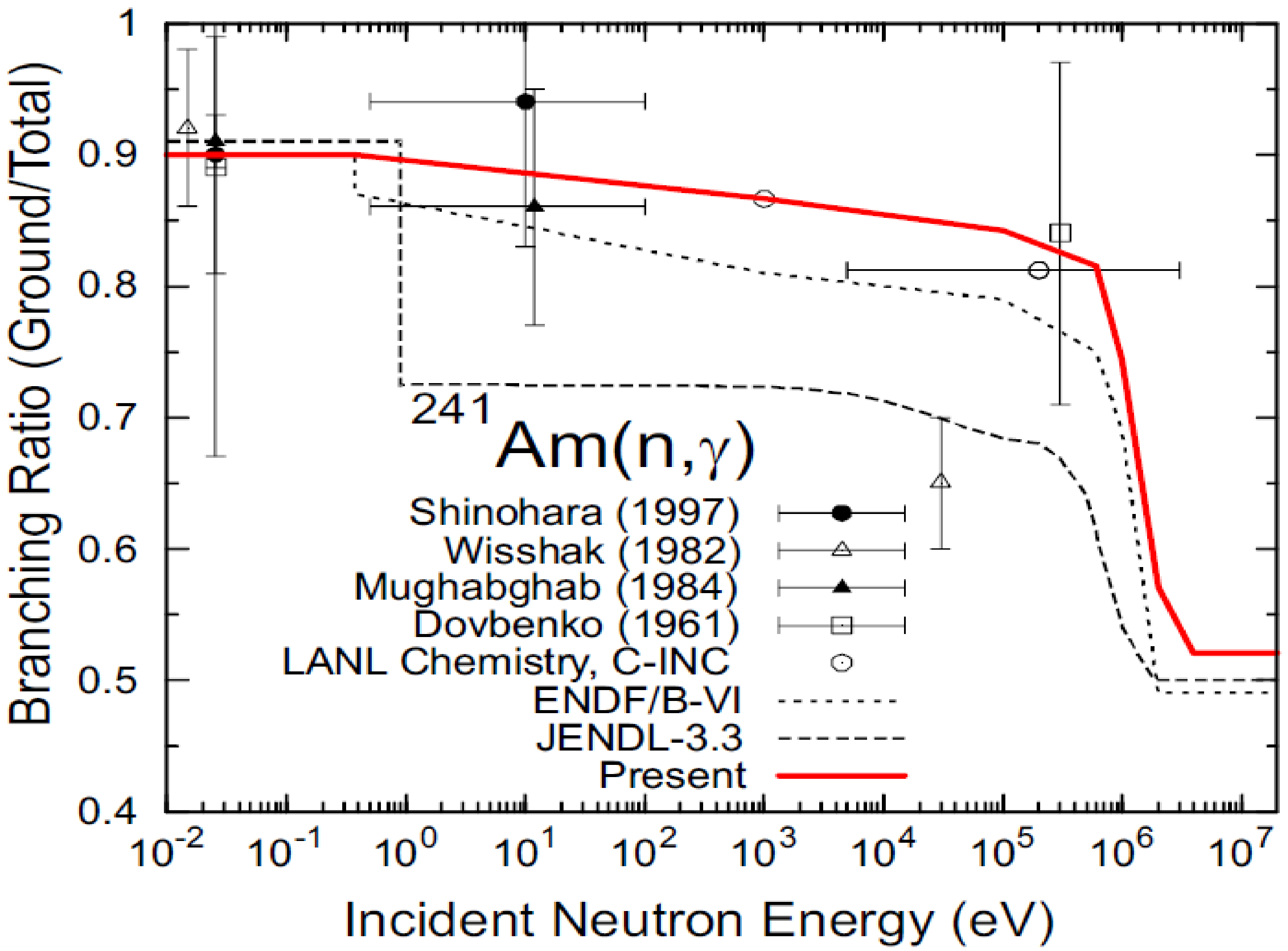
Michael J. Eades, et al., The influence of Xe-135m on steady-state xenon worth in thermal molten salt reactors, Progress in Nuclear Energy 93 (2016).

Analysis found it doesn't really matter for LWR because fraction of Xe135m is small at power → after 1 hr. decay → all Xe-135

Missing Data: Am-241 + n → γ + Am-242/Am-242m

^{242m}Am $T_{1/2}$ = 114 y
^{242}Am $T_{1/2}$ = 16 h

- Neutron transport does not care about daughter products
- **Depletion does!** spectrum-dependent assumption of 85% vs. 88% can induce a "measurable" error



Unexpected Uncertainty:

- Delayed neutron fraction, arguably one of most important safety parameters

$$\frac{dn(t)}{dt} = \frac{\rho - \beta_{eff}}{\Lambda} n(t) + \sum_{i=1}^{N} \lambda_i C_i(t)$$

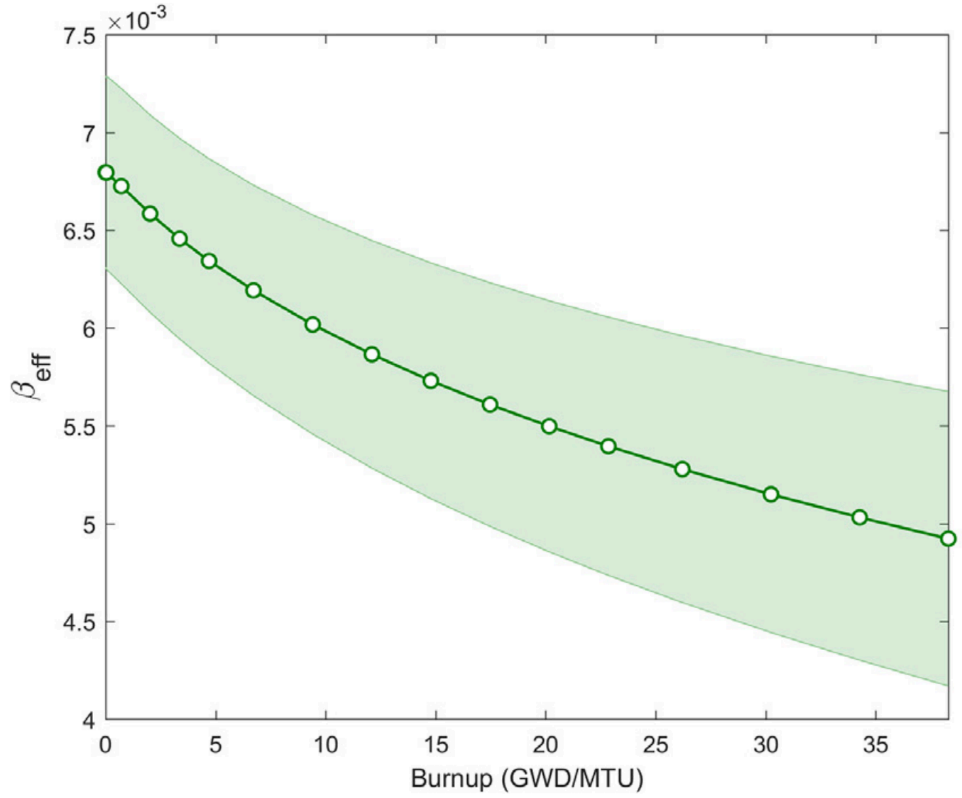
$$\frac{dC_i(t)}{dt} = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t), \qquad (i = 1, \ldots, N)$$

- **For LWR systems**: SCALE/Sampler uncertainty propagation of just **cross sections**
  - Fresh fuel: β_{eff}~700 pcm +/- 7%
  - 40 GWd/MTU: β_{eff} ~500 pcm +/- 15% (2-sigma range is 350-650 pcm)

- Is it real?
  - Sampling error?
  - Neglected correlation?
  - **As we investigate non-LWRs, need perspective**

$$\beta_{eff} = \sum_{i=1}^{6} \frac{\sum_j \sum_m V_m \left(\sum_g \nu\sigma_{fjgm} n_{jm} \phi_{m,g}\right)\left(\sum_{g'} \beta_{g'ji}\, \chi_{d,g'mj} \phi^*_{g'm}\right)}{\sum_j \sum_m V_m \left(\sum_g \nu\sigma_{fjgm} n_{jm} \phi_{m,g}\right)\left(\sum_{g'} \bar{\chi}_{g'mj} \phi^*_{g'm}\right)}$$

j – fissionable nuclide
m – material
i – delayed neutron group

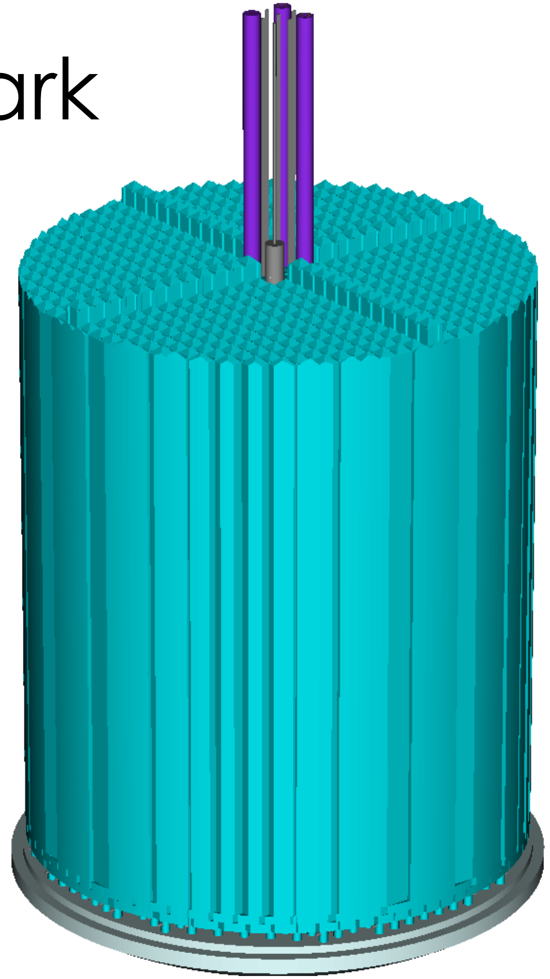


Majdi I. Radaideh, William A. Wieselquist, Tomasz Kozlowski, "A new framework for sampling-based uncertainty quantification of the six-group reactor kinetic parameters", *Annals of Nuclear Energy*, Volume **127** (2019).

Potential Nuclear Data Gap: MSRE Benchmark

New IRPHE Benchmark has reference model with
keff ~ 0.99978 +/- 0.00400

- Benchmark Serpent and recent SCALE model has ~1.02
- Limited MSR validation data so need to use MSRE but have 2000 pcm bias with +/- 400 pcm uncertainty
  - Is there unaccounted for model/experiment uncertainty?
  - **Is this a nuclear data/code bias?**



Confidence in SCALE non-LWR criticality predictions is very important for future NRC confirmatory/licensing analysis!