# Validation Efforts TRITON to NESTLE Integration


**ORNL**

**26-May-2009**

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THE UNIVERSITY of TENNESSEE KNOXVILLE

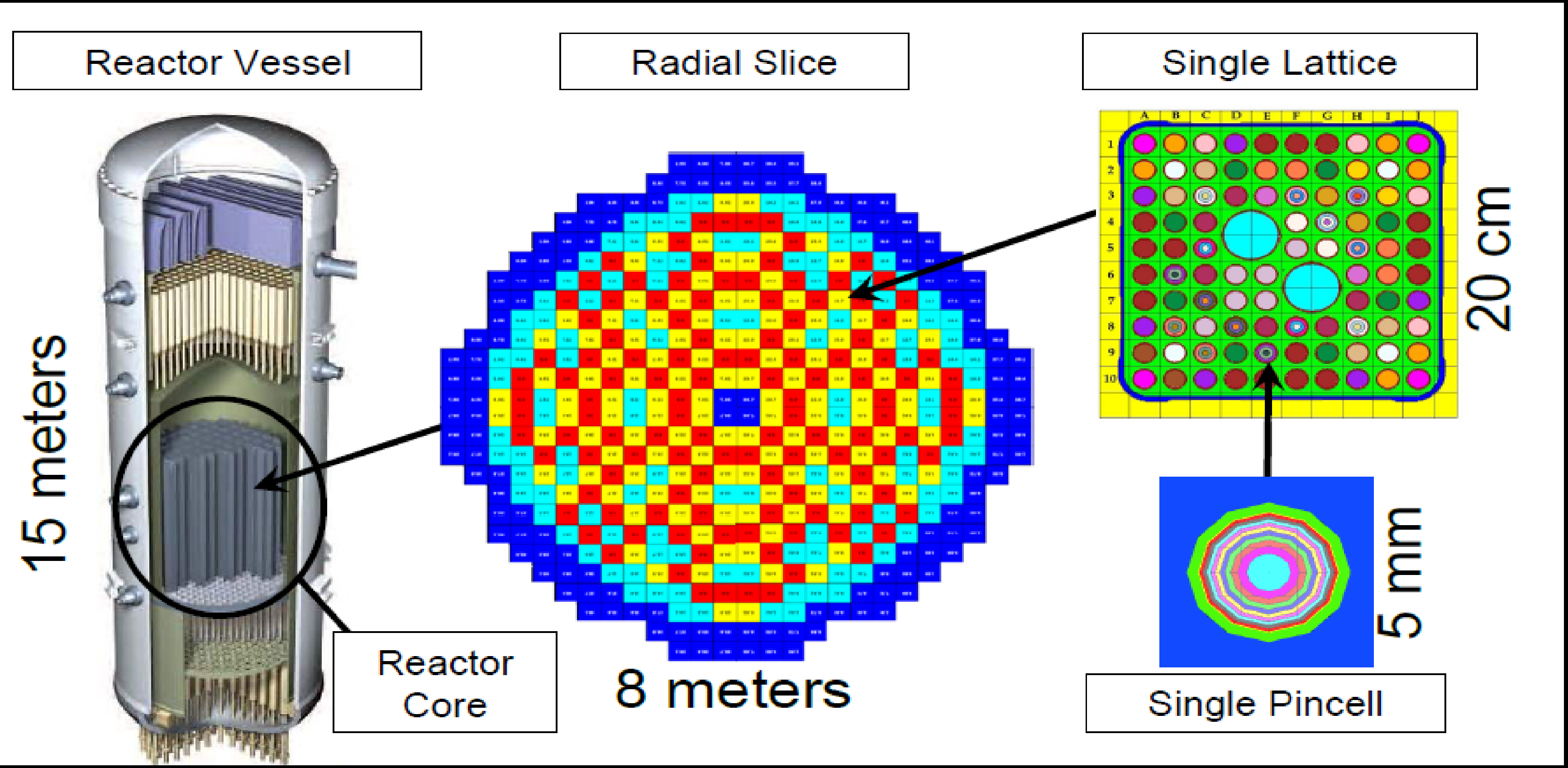
# Chavers Biography

- University of Tennessee
- Nuclear Engineering
- Seven Semesters with Southern Nuclear in Core Analysis and Design
- NESLS Spring 2009
  - NESTLE Seed Project
  - Mentor:  Kevin Clarno
  - UT Major Advisor:  Ivan Maldonado

# Outline

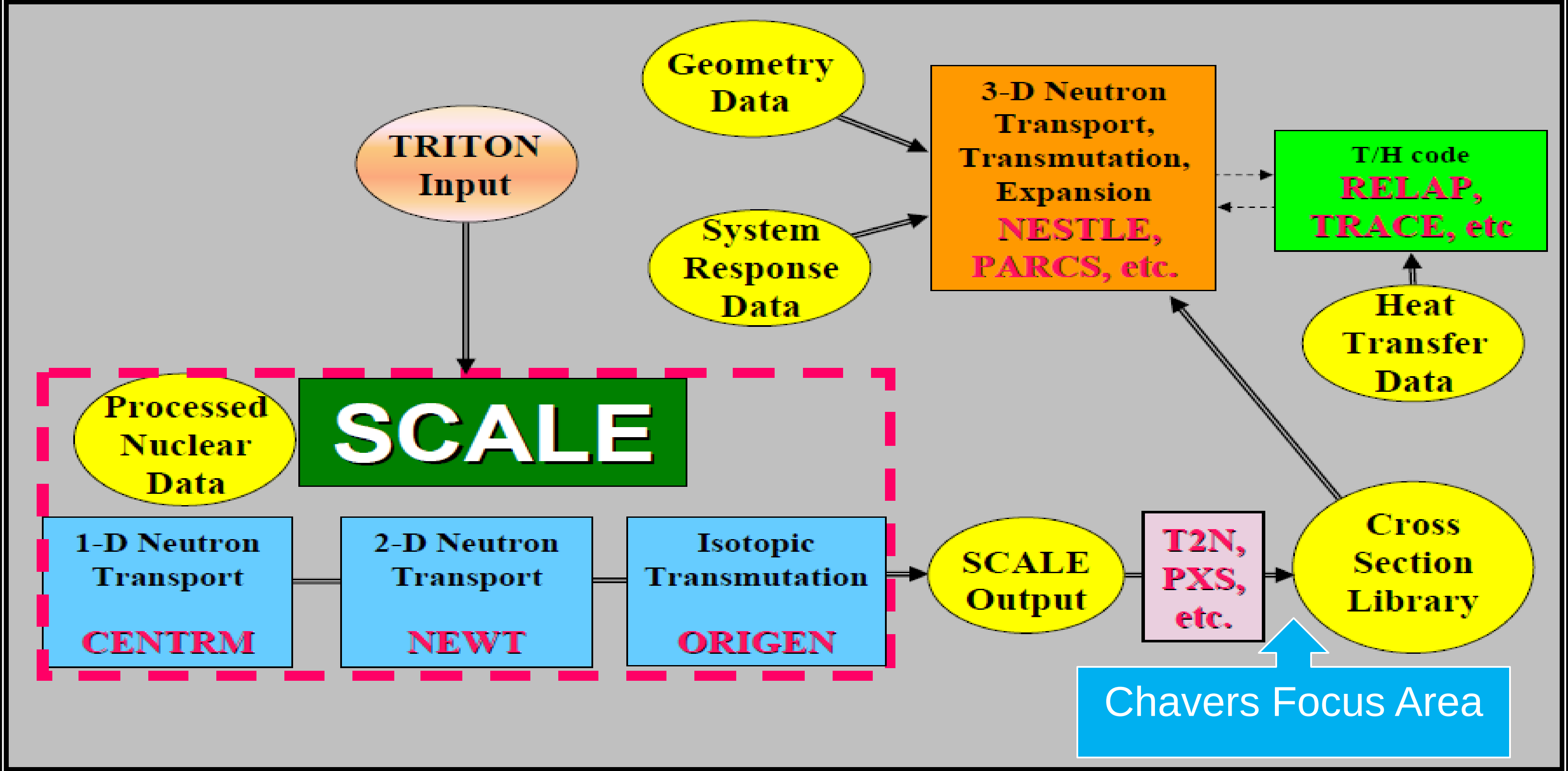
- Background on HOW reactor simulation is done
- Discussion of the NESTLE Seed Project
- TRITON to NESTLE Integration
  - Simple PWR Model
  - Simple BWR Model
  - Peach Bottom Cycle 1

# Background: Hierarchical Structure



# Background:

## End-to-End Reactor Analysis with Open Source Code



# NESTLE SEED PROJECT

- NESTLE
  - **N**odal **E**igenvalue, **S**teady-State, **T**ransient, **L**e core **E**valuator
  - Few Group Neutron Diffusion Equation Solver for Steady-State and Transient Problems
  - Geared specifically toward full core analysis of nuclear reactors
  - Developed by North Carolina State University

# NESTLE SEED PROJECT

- NESTLE SEED PROJECT
  - Kevin Clarno, Matt Jessee, Ivan Maldonado, Emilian Popov
  - HOST of UT Volunteers: J. Galloway, H. Hernandez, J. Chavers, M. Masse (now MIT), S. McKee (now MIT)
- Modularize and Incorporate into the SCALE package
  - Matt Jessee (Lead), H. Hernandez, J. Chavers
  - Includes: Automation of cross section data transference between TRITON and NESTLE
- BWR Compatibility
  - Emilian Popov (Lead), J. Galloway
  - Includes: Developing New Drift-Flux Component
- Microscopic Depletion
  - Including the utilization of CILO file

# Methodology
## A SCALE input deck looks like…..

- =T-DEPL (TRITON)
  - Creates Inputs for all the functional codes to develop cross sections for use in full core solver
    - (BONAMI, CENTRM, PMC, NEWT, ORIGEN-S, etc)
    - Expanded Capability to run Branch Cases in Parallel
- =T2N
  - Interface code reads TRITON xfile016 to generate cross section input to NESTLE
- =NESTLE
  - Few Group Neutron Diffusion Equation Solver for Steady-State and Transient Problems

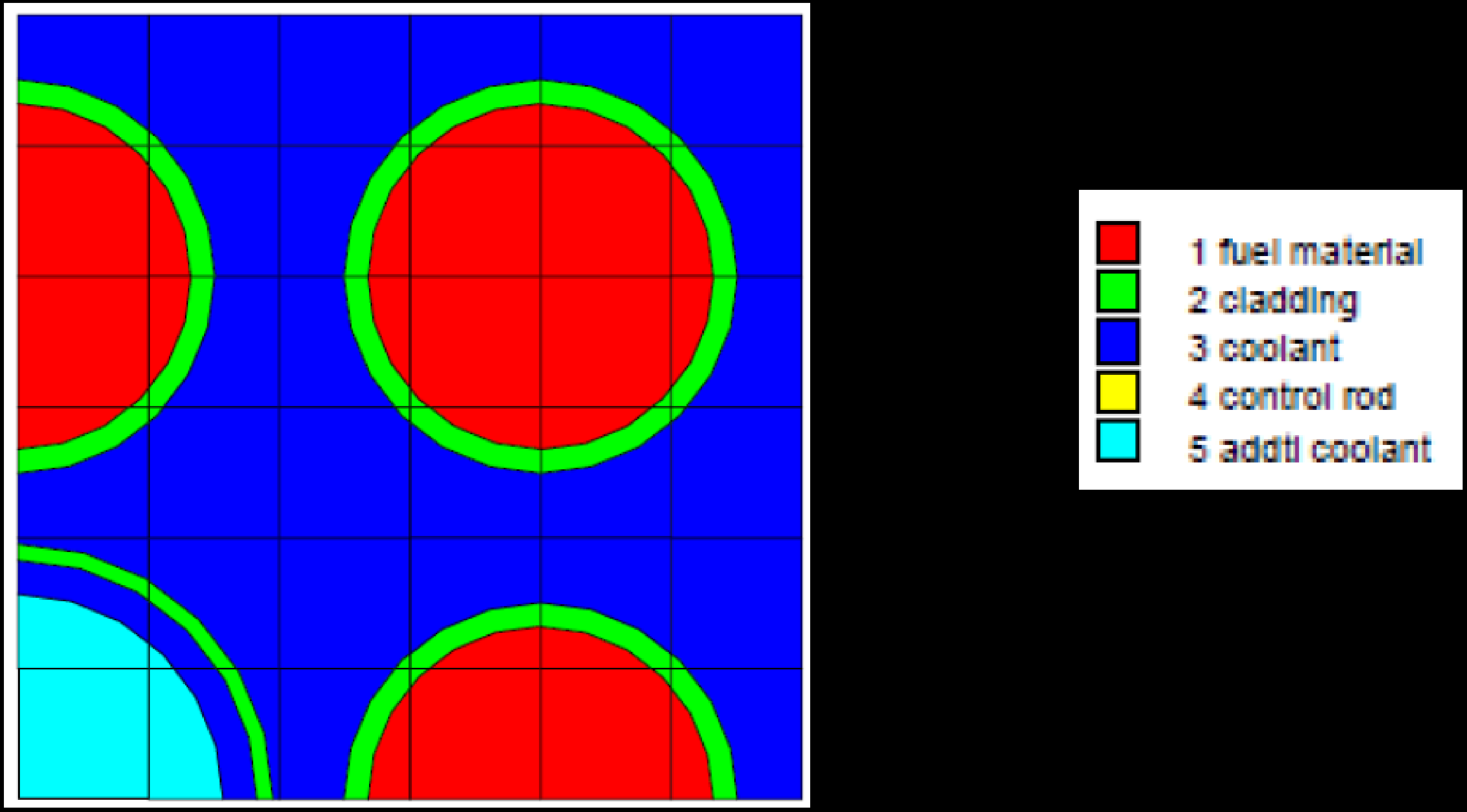
# Objectives

- Simple PWR Model
  - Originally Developed by S. Mckee (MIT) and K. Clarno
  - Modularized previous model to the =TRITON, =T2N, =NESTLE input format
  - Use Model to Perform Validation Efforts to TRITON To NESTLE Integration
- Simple BWR Model
  - Develop BWR model in similar scope to Simple PWR Model to validate unique features of the BWR
- Peach Bottom BWR
  - Revise Existing TRITON input decks used for PARCS
  - Develop =NESTLE inputs structure and geometry (Chavers, Galloway)

# Challenges
## Major Challenges encountered….

- SCALE6.dev – TRITON
  - Developmental Code is in a continuous evolutionary process that make reproducing results challenging.
  - What is the correct answer this week?
- T2N
  - Dependency on TRITON output results in high degree of sensitivity to changes in xfile016. (SCALE6 vs SCALE6.dev)
- NESTLE
  - Code is still in Development - BWRs
  - Based entirely N. C. State student coding….
    - Bugs
    - Inconsistencies
    - Not Developer Friendly

# Simple PWR Model
## Based on Turkey Point Unit 3



# Simple PWR Model
## Based on Turkey Point Unit 3

**Table 1: Model Parameters, Based on Turkey Point Unit 3 [DeHart, 1996]**

| | |
|---|---|
| Assembly type | Westinghouse 15 x 15 |
| Number of fuel rods | 204 |
| Number of guide tubes | 20 |
| Number of instrument tubes | 1 |
| Rod pitch | 1.43 cm |
| Rod OD | 1.0719 cm |
| Rod ID | 0.9484 cm |
| Pellet OD | 0.9296 cm* |
| Control rod OD | 1.1162 cm |
| Average fuel temperature | 922 K |
| Average clad temperature | 595 K |
| Average coolant temperature | 570 K |

*Not used in present work due to use of reduced density fuel

# Simple PWR Model
## Based on Turkey Point Unit 3

**Table 2: Uranium Isotopic Composition, from Turkey Point Unit 3 [DeHart, 1996]**

| Isotope | wt% |
|---|---|
| $^{234}U$ | 0.023 |
| $^{235}U$ | 2.556 |
| $^{236}U$ | 0.012 |
| $^{238}U$ | 97.409 |

# Simple PWR Model
## Initial Results….

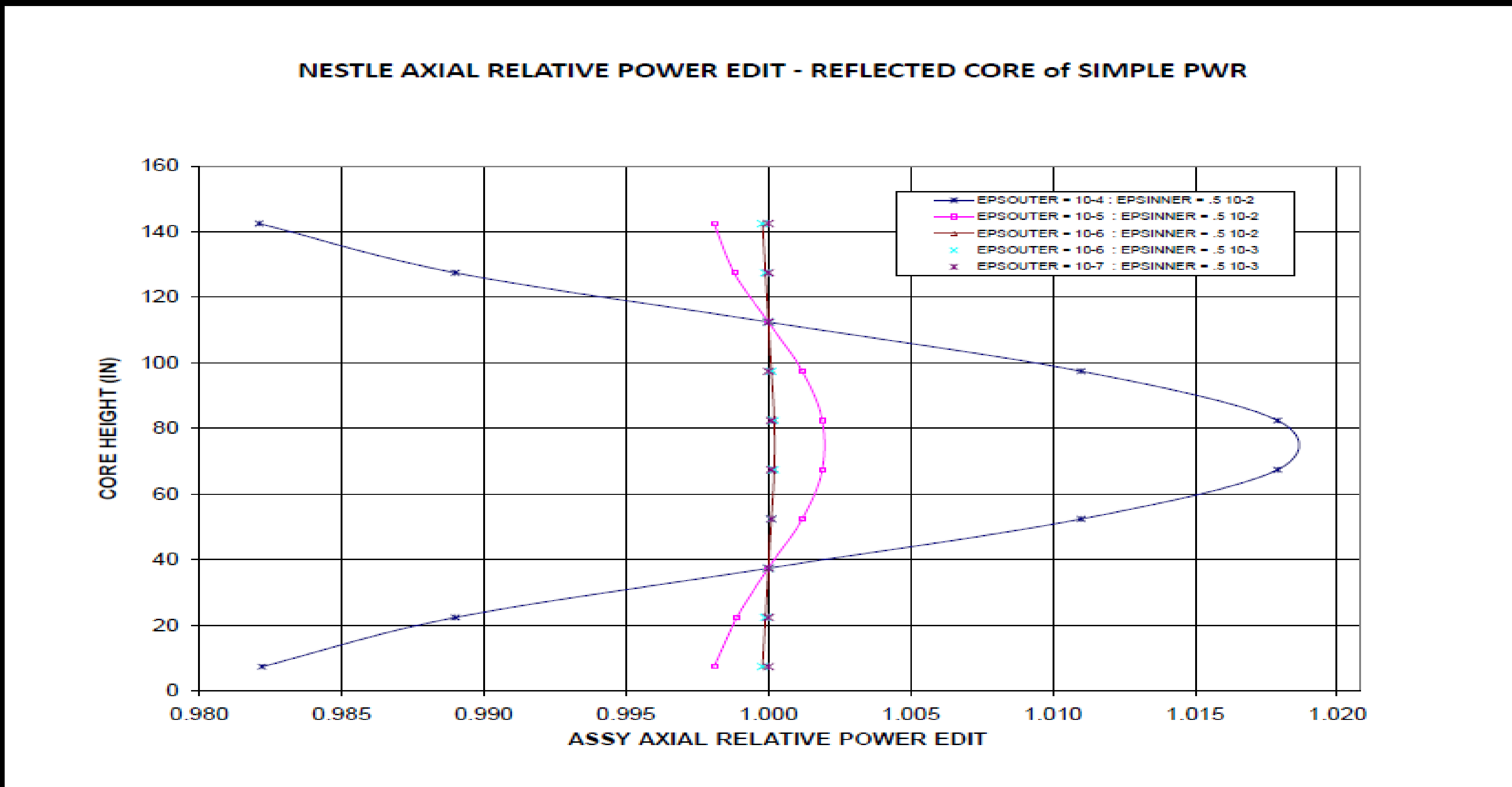
| SIMPLE PWR - Results from McKee Report | | | |
|---|---|---|---|
| Burnup | TRITON | NESTLE | PCM Difference |
| *MWD/MT* | *k-inf* | *k-inf* | *pcm* |
| 0 | 1.304895 | 1.29399 | 1090.7 |
| 30 | 1.266587 | 1.24453 | 2205.4 |
| 230 | 1.261075 | 1.24272 | 1835.2 |
| 500 | 1.253635 | 1.24028 | 1335.7 |
| 795 | 1.245507 | 1.23762 | 789 |
| 1295 | 1.239462 | 1.23193 | 753.6 |
| 2265 | 1.220944 | 1.22085 | 9.9 |
| 3250 | 1.207563 | 1.20753 | 2.9 |
| 5250 | 1.180982 | 1.18144 | -45.5 |
| 7250 | 1.15617 | 1.15683 | -65.8 |
| 9250 | 1.131357 | 1.13289 | -153.3 |
| 10750 | 1.114913 | 1.11614 | -122.2 |
| 11750 | 1.10395 | 1.10534 | -139.4 |
| 12500 | 1.095728 | 1.09705 | -132.2 |

Not Good!

# A Plan of Action….
## Zero Exposure Must be Equal!

- Verify TRITON $K_{inf}$ with Hand Calculations
- Verify T2N Cross Section Processing
  - Indentified and Corrected Issues
    - Group 2 Cross Sections Imported Incorrectly
    - T2N incompatibility with up-scatter
    - General shifts in cross section data with modifications to TRITON output
    - Coefficient cross section calculations – based on branch cases
- NESTLE
  - NEM – Convergence : Utilize: fdm
  - $K_{inf}$ with a power shape?
  - Tighten convergence Criteria

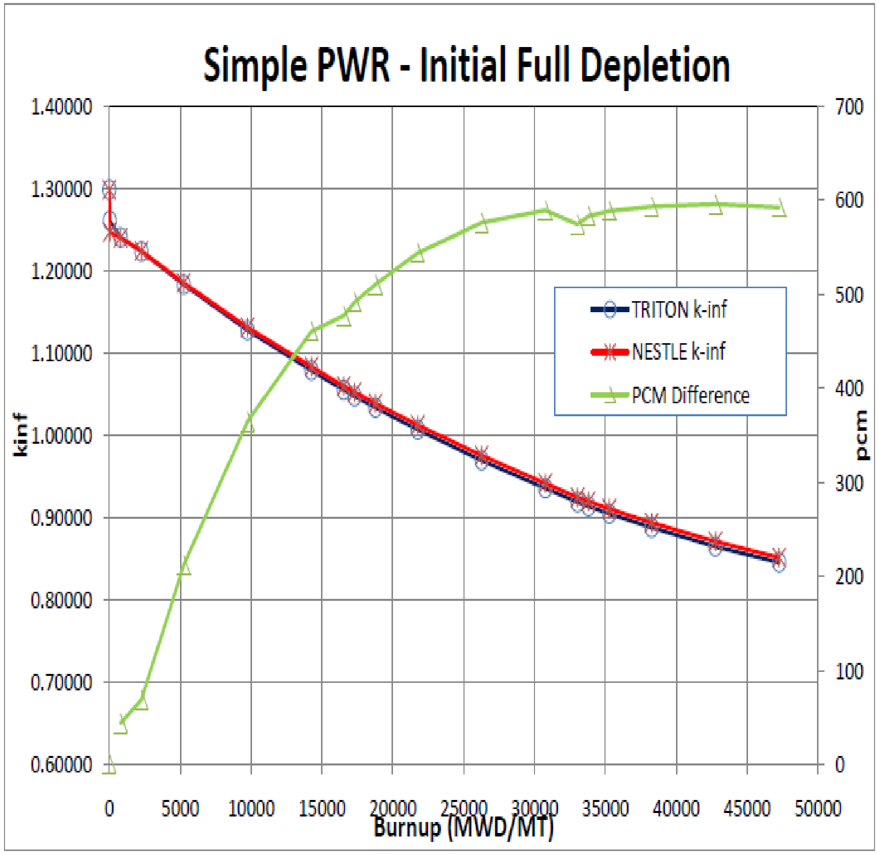
# Simple PWR Model
## with Reflective Condition at all boundaries…



# Simple PWR Model
## with corrections…

| Simple PWR Model at 0.0 MWD/MT | | | |
|---|---|---|---|
| Source | TRITON | NESTLE | PCM Difference |
| | *k-inf* | *k-inf* | *pcm* |
| Original SCALE6 @ 238group | 1.30499 | 1.29205 | 1294 |
| Optimized NEWT/TRITON @ 44group | 1.29832 | 1.29830 | 1.8 |
| Optimized NEWT/TRITON @ 49group | 1.30281 | 1.30281 | 0.3 |
| Optimized NEWT/TRITON @ 238group | 1.30476 | 1.30445 | 30.6 |
| SCALE6.dev Parallel @ 44group | 1.29852 | 1.29853 | -0.3 |
| SCALE6.dev Parallel @ 49group | 1.30281 | 1.30271 | 9.9 |
| SCALE6.dev Parallel @ 238group | 1.30477 | 1.30437 | 39.8 |
| NOTES: Fast-Thermal Boundary 0.625 eV | | | |

# Simple PWR Model Depletion Cases




| SIMPLE PWR - Initial Full Depletion | | | |
|---|---|---|---|
| Burnup | TRITON | NESTLE | PCM Difference |
| *MWD/MT* | *k-inf* | *k-inf* | *pcm* |
| 0 | 1.29832 | 1.29830 | 1.8 |
| 30 | 1.26071 | 1.24687 | 1383.7 |
| 795 | 1.24032 | 1.23987 | 44.5 |
| 2265 | 1.22321 | 1.22391 | -69.6 |
| 5250 | 1.18325 | 1.18537 | -212.3 |
| 9750 | 1.12766 | 1.13131 | -365 |
| 14250 | 1.07906 | 1.08367 | -460.6 |
| 16530 | 1.05515 | 1.05992 | -477.3 |
| 17295 | 1.04775 | 1.05266 | -491.4 |
| 18765 | 1.03388 | 1.03898 | -510.5 |
| 21750 | 1.00724 | 1.01268 | -543.6 |
| 26250 | 0.96995 | 0.97571 | -576 |
| 30750 | 0.93608 | 0.94197 | -589 |
| 33030 | 0.91920 | 0.92494 | -574.3 |
| 33795 | 0.91429 | 0.92012 | -582.9 |
| 35265 | 0.90523 | 0.91111 | -588.3 |
| 38250 | 0.88827 | 0.89420 | -593 |
| 42750 | 0.86537 | 0.87133 | -595.6 |
| 47250 | 0.84600 | 0.85192 | -592.2 |

NOTE: 44group Optimized Execution

# Simple PWR Model

## TRITON Nuclide Control Options (ADDNUX=1)

Utilize TRITON's unique nuclide control option to determine if fission products are underlying issue.  ADDNUX=1 recognizes only 16 nuclides (actinides).

| | | | |
|---|---|---|---|
| 1/v Absorber | $^{234}U$ | $^{235}U$ | $^{236}U$ |
| $^{238}U$ | $^{237}Np$ | $^{238}Pu$ | $^{239}Pu$ |
| $^{240}Pu$ | $^{241}Pu$ | $^{242}Pu$ | $^{241}Am$ |
| $^{242}Am$ | $^{243}Am$ | $^{242}Cm$ | $^{243}Cm$ |

# Simple PWR Model Nuclide Control Case

- Verify Xe and Sm Cross Sections
- Verify Fission Product Yields
  - I-135
  - Xe-235
  - Pm-149

| SIMPLE PWR - DEPLETION with Nuclide Control Imposed | | | |
|---|---|---|---|
| Burnup | TRITON | NESTLE | PCM Difference |
| *MWD/MT* | *k-inf* | *k-inf* | *pcm* |
| 0 | 1.298524 | 1.298527 | -0.3 |
| 30 | 1.298384 | 1.298386 | -0.2 |
| 795 | 1.295036 | 1.295027 | 0.9 |
| 2265 | 1.284340 | 1.284352 | -1.2 |
| 5250 | 1.255333 | 1.255329 | 0.4 |
| 9750 | 1.212565 | 1.212564 | 0.1 |
| 14250 | 1.173672 | 1.173660 | 1.2 |
| 16530 | 1.153063 | 1.153051 | 1.2 |
| 17295 | 1.146861 | 1.146853 | 0.8 |
| 18765 | 1.135064 | 1.135060 | 0.4 |
| 21750 | 1.112226 | 1.112212 | 1.4 |
| 26250 | 1.079099 | 1.079096 | 0.3 |
| 30750 | 1.047466 | 1.047449 | 1.7 |
| 33030 | 1.030133 | 1.030126 | 0.7 |
| 33795 | 1.025349 | 1.025350 | -0.1 |
| 35265 | 1.016478 | 1.016466 | 1.2 |
| 38250 | 1.000216 | 1.000200 | 1.6 |
| 42750 | 0.978249 | 0.978254 | -0.5 |
| 47250 | 0.959498 | 0.959537 | -3.9 |

# A Plan of Action….

- Yields were assumed constant in T2N

  - I-135: 0.63800E-01
  - Xe-135: 0.228000E-02
  - Pm-149: 0.113000E-01

- Request that TRITON provide yields on xfile016
- ……TRITON yields provided are orders of magnitude different from expected values for Pm-149 and Xe-235

# A Plan of Action….

## Reverse Calculate Yields

- NESTLE Manual Section II.7.a discusses treatment of fission products that effectively correct absorption cross sections.

- Required Assumptions
  - Suppress Spatial Dependence
  - Assume Steady State Equilibrium Conditions
  - Assume I-135 Yield from TRITON is correct

# A Plan of Action….

## Reverse Calculate - Iodine-Xenon Chain

$$\frac{d}{dt}N_I^l(t) = \gamma_I^l \sum_{g=1}^{G} \Sigma_{f_g}^l(t)\phi_g^l(t) - \lambda_I^l N_I^l(t)$$

$$\frac{d}{dt}N_{Xe}^l(t) = \lambda_I^l N_I^l(t) + \gamma_{Xe}^l \sum_{g=1}^{G} \Sigma_{f_g}^l(t)\phi_g^l(t) - \lambda_{Xe}^l N_{Xe}^l(t) - \sum_{g=1}^{G} \sigma_{Xe_{ag}}^l(t)\phi_g^l(t) N_{Xe}^l(t)$$

$$N_{I_\infty}^l = \frac{\gamma_I^l \sum_{g=1}^{G} \Sigma_{f_g}^l \phi_g^l}{\lambda_I}$$

$$\gamma_{Xe}^l = \frac{\lambda_{Xe}^l N_{Xe_\infty}^l + \sum_{g=1}^{G} \sigma_{Xe_{ag}}^l \phi_g^l N_{Xe_\infty}^l(t) - \lambda_I^l N_{I_\infty}^l}{\sum_{g=1}^{G} \Sigma_{f_g}^l \phi_g^l}$$

# A Plan of Action….

## Reverse Calculate – Promethium-Samarium Chain

$$\frac{d}{dt}N_{Pm}^{l}(t) = \gamma_{Pm}^{l}\sum_{g=1}^{G}\Sigma_{f_g}^{l}(t)\phi_g^{l}(t) - \lambda_{Pm}^{l}N_{Pm}^{l}(t)$$

$$\frac{d}{dt}N_{Sm}^{l}(t) = \lambda_{Pm}^{l}N_{Pm}^{l}(t) - \sum_{g=1}^{G}\sigma_{Sm_{ag}}^{l}(t)\phi_g^{l}(t)N_{Sm}^{l}(t)$$

$$N_{Pm_\infty} = \frac{N_{Sm_\infty}\sum_{g=1}^{G}\sigma_{Sm_{ag}}^{l}\phi_g^{l}}{\lambda_{Pm}}$$

$$\gamma_{Pm}^{l} = \frac{N_{Pm_\infty}\lambda_{Pm}}{\sum_{g=1}^{G}\Sigma_{f_g}^{l}\phi_g^{l}}$$

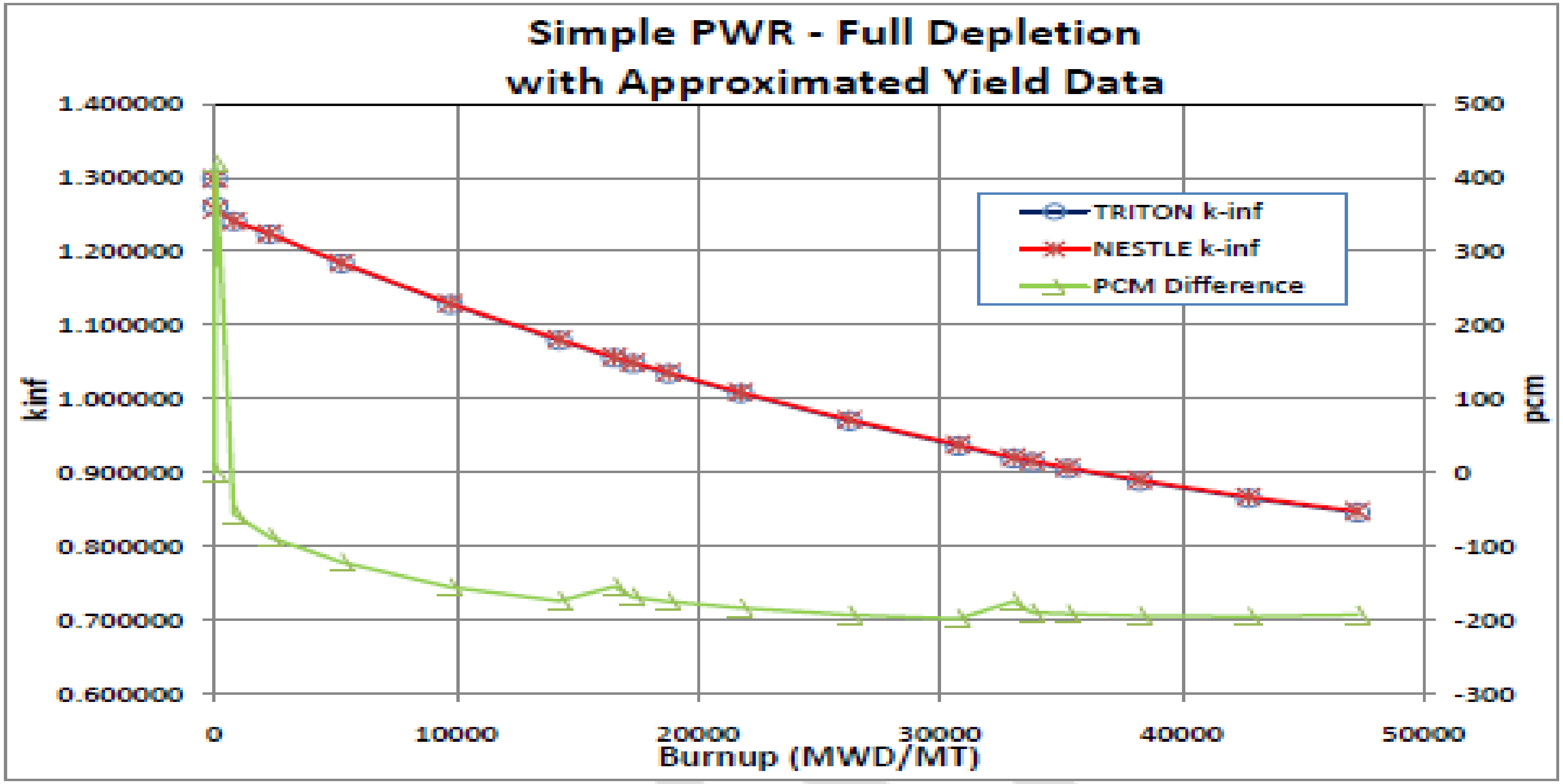
# Simple PWR Model
## Full Depletion Model

- Small Divergence due to Assumption of Steady State Condition

| SIMPLE PWR - SCALE6.dev RUN at 44 group | | | |
|---|---|---|---|
| Burnup | TRITON | NESTLE | PCM Difference |
| *MWD/MT* | *k-inf* | *k-inf* | *pcm* |
| 0 | 1.298524 | 1.298527 | -0.3 |
| 30 | 1.260947 | 1.256759 | 418.8 |
| 795 | 1.240578 | 1.241140 | -56.2 |
| 2265 | 1.223463 | 1.224337 | -87.4 |
| 5250 | 1.183445 | 1.184661 | -121.6 |
| 9750 | 1.127828 | 1.129381 | -155.3 |
| 14250 | 1.079197 | 1.080936 | -173.9 |
| 16530 | 1.055292 | 1.056838 | -154.6 |
| 17295 | 1.047884 | 1.049573 | -168.9 |
| 18765 | 1.033996 | 1.035745 | -174.9 |
| 21750 | 1.007336 | 1.009171 | -183.5 |
| 26250 | 0.969968 | 0.971897 | -192.9 |
| 30750 | 0.936038 | 0.938018 | -198 |
| 33030 | 0.919179 | 0.920928 | -174.9 |
| 33795 | 0.914270 | 0.916167 | -189.7 |
| 35265 | 0.905193 | 0.907107 | -191.4 |
| 38250 | 0.888221 | 0.890163 | -194.2 |
| 42750 | 0.865304 | 0.867254 | -195 |
| 47250 | 0.845911 | 0.847839 | -192.8 |

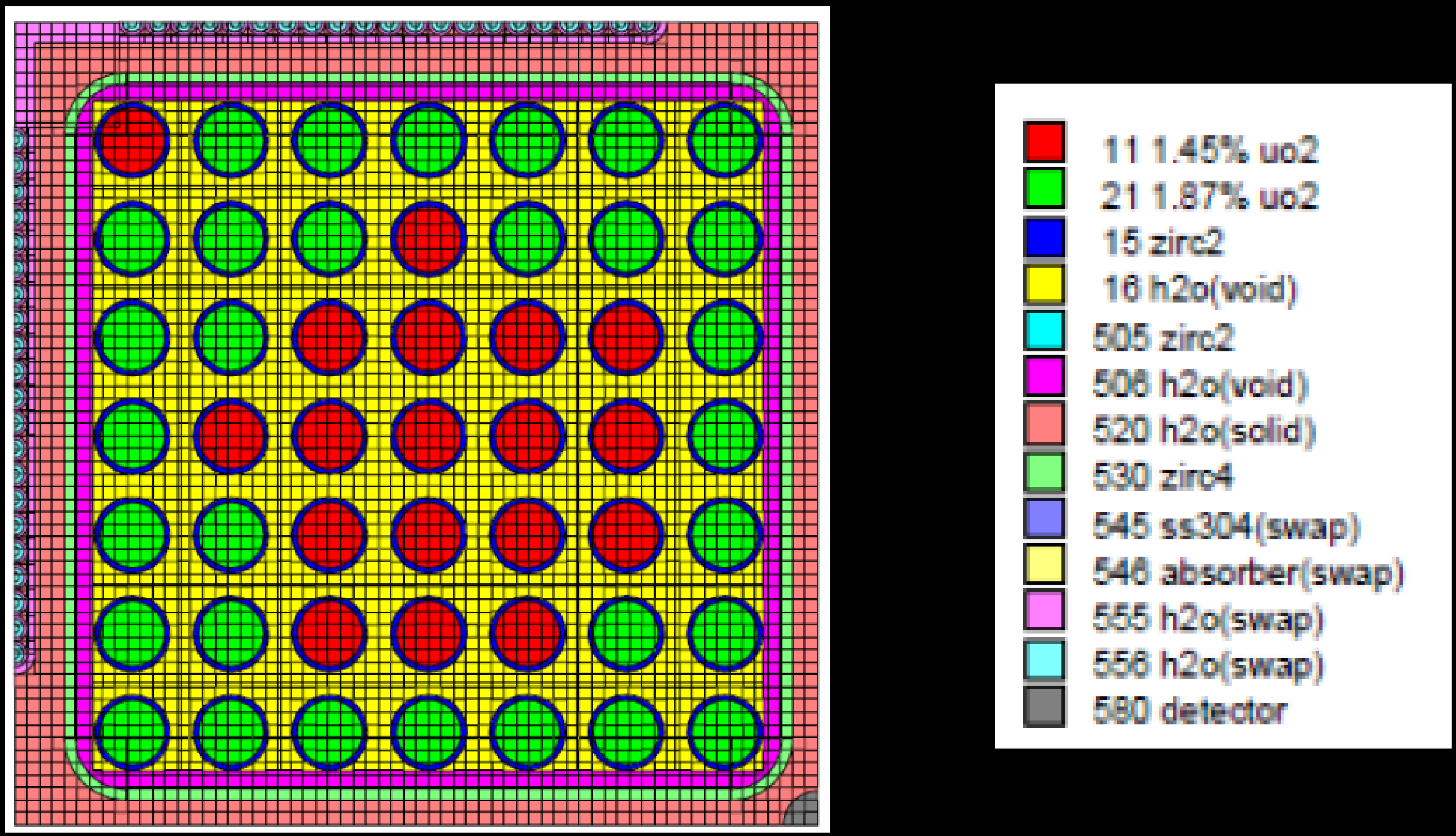
# Simple PWR Model

## Full Depletion Model – with approximated yields



# Simple BWR Model

## Based on Peach Bottom Cycle 1 Fuel Type 1



# Simple BWR Model
## Special Consideration with TRITON / NEWT

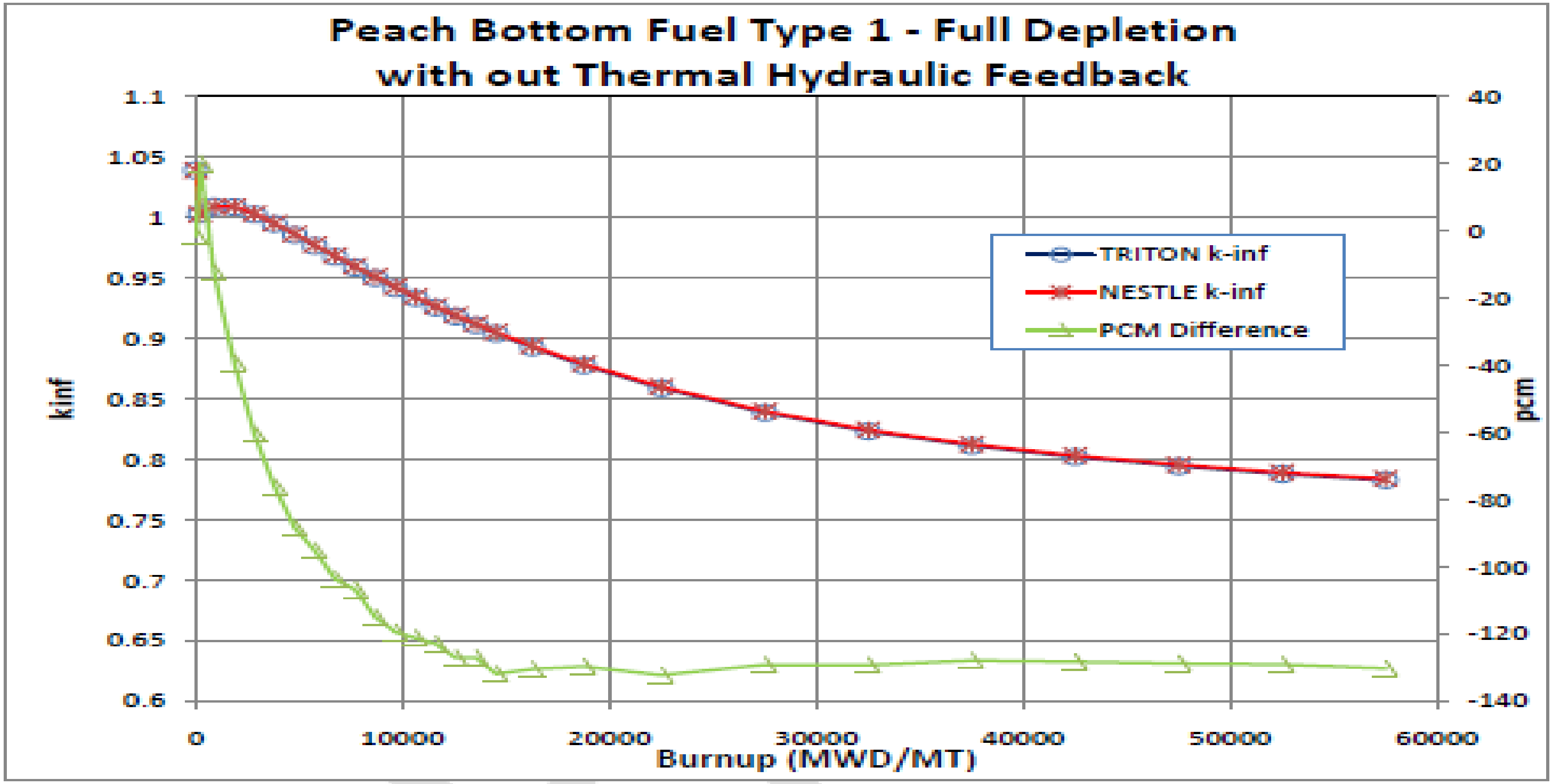
- More Complex Geometry requires increased mesh
  - Increases computational time
  - parm=check before execution
- Lessons Learned:
  - “Tracer Error:  Mesh Too Course”  - Increase the number of sides used to approximate a cylinder (sides=24)
  - Best Results Produced with:
    - Sn=8    inners=6    outers=200    cmfd= yes    xycmfd=8
    - epsinner=1e-7    epsouter=1e-6    epsilon=1e-5
    - Pin Boundary:  1x1            Global Boundary:  64x64

# BWR Model
## Full Depletion Model

- Similar Trend to Simple PWR Full Depletion Model

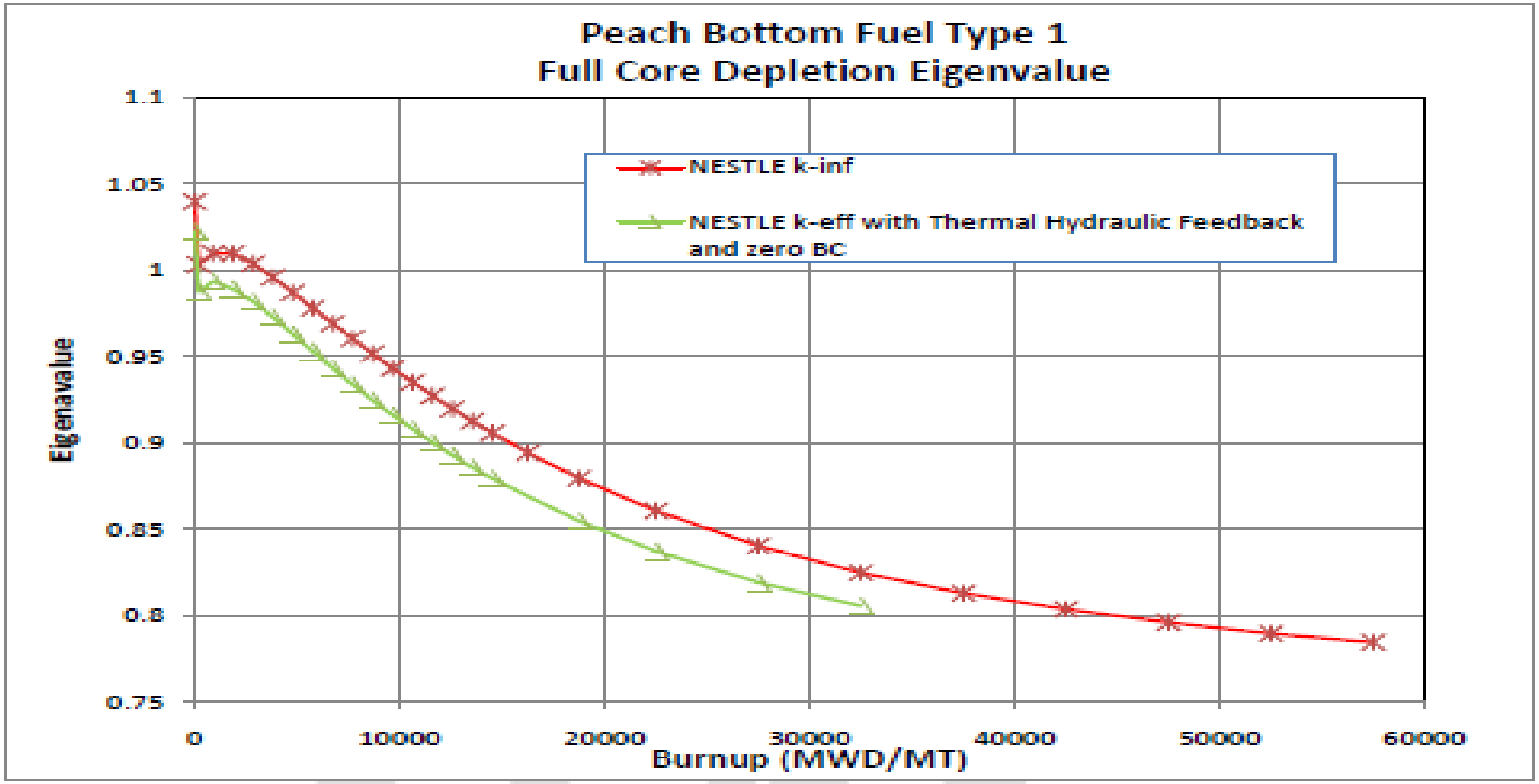
| Peach Bottom Fuel Type 1 | | | |
|---|---|---|---|
| Burnup | TRITON | NESTLE | PCM Difference |
| *MWD/MT* | *k-inf* | *k-inf* | *pcm* |
| 0 | 1.039315 | 1.03933 | -1.5 |
| 200 | 1.003213 | 1.00301 | 20.3 |
| 887 | 1.009367 | 1.00949 | -12.3 |
| 1860 | 1.008988 | 1.00938 | -39.2 |
| 2833 | 1.003026 | 1.00363 | -60.4 |
| 3807 | 0.9949 | 0.99566 | -76 |
| 4780 | 0.985986 | 0.98687 | -88.4 |
| 5753 | 0.976849 | 0.9778 | -95.1 |
| 6727 | 0.967894 | 0.96893 | -103.6 |
| 7700 | 0.959013 | 0.96008 | -106.7 |
| 8673 | 0.950311 | 0.95146 | -114.9 |
| 9647 | 0.941846 | 0.94304 | -119.4 |
| 10620 | 0.933689 | 0.9349 | -121.1 |
| 11593 | 0.925841 | 0.92707 | -122.9 |
| 12567 | 0.91831 | 0.91958 | -127 |
| 13540 | 0.91111 | 0.91238 | -127 |
| 14513 | 0.904242 | 0.90556 | -131.8 |
| 16250 | 0.892826 | 0.89413 | -130.4 |
| 18750 | 0.877854 | 0.87915 | -129.6 |
| 22500 | 0.859118 | 0.86044 | -132.2 |
| 27500 | 0.838819 | 0.84011 | -129.1 |
| 32500 | 0.823358 | 0.82465 | -129.2 |
| 37500 | 0.811512 | 0.81279 | -127.8 |
| 42500 | 0.802178 | 0.80346 | -128.2 |
| 47500 | 0.794563 | 0.79585 | -128.7 |
| 52500 | 0.78814 | 0.78943 | -129 |
| 57500 | 0.783028 | 0.78433 | -130.2 |

# Simple BWR Model
## Full Depletion Model – Peach Bottom Fuel Type 1



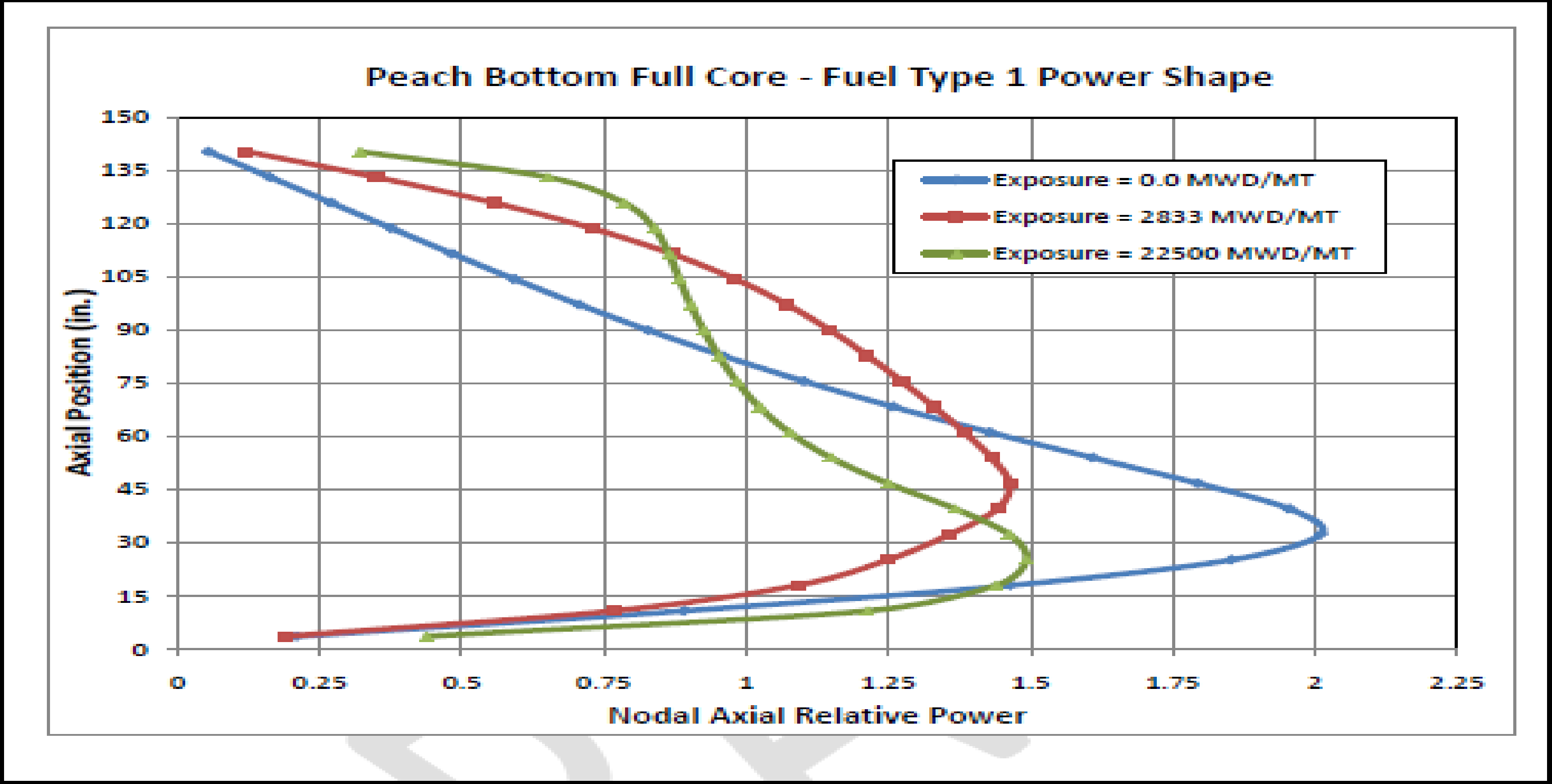
# Simple BWR Model

## Full Depletion Model with new Drift-Flux Component



# Simple BWR Model

## Full Depletion Model Power Shape



# Peach Bottom

## Status Update on Cycle 1 Full Core Model

- Three Fuel Types
  - Total of 8 Fuel Lattices each with 8 Branch Calculations
  - 0%, 20%, 40%, 60%, 80% voiding
  - Parallel Execution decreases execution time from 8 days to ~23 hours
  - Cross Sections generation nearing completion

- Core Geometry model is being developed for NESTLE

# Future Work

- Utilization of microscopic cross sections for use in NESTLE – Cilo File
- Continued Benchmarking with Peach Bottom Cycle 1 for BWR code components
- Further Benchmarking against existing core simulators

# Conclusions

- Macroscopic cross section processing in T2N is being performed correctly
- Initial BWR results show promising results in regards to BWR performance
- Further Benchmarking is required

# Questions?

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