INL/JOU-16-40110-Revision-0

Combining RAVEN, RELAP5-3D and PHISICS for Fuel Cycle and Core Design Analysis for New Cladding Criteria

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March 2017

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Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
U.S. Department of Energy

Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

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Dr. Andrea Alfonsi
Idaho National Laboratory
2525 Fremont Ave
Idaho Falls, ID, 83402
Andrea.Alfonsi@inl.gov

Dr. George L Mesina
Idaho National Laboratory
2525 Fremont Ave
Idaho Falls, ID, 83402
George.Mesina@inl.gov
ASME Membership

Angelo Zoino
University La Sapienza
Rome, 00135, Italy
angelo@zoino.it

Nolan Anderson
Idaho National Laboratory
2525 Fremont Ave
Idaho Falls, ID, 83402
Nolan.Anderson@inl.gov

Dr. Cristian Rabiti
Idaho National Laboratory
2525 Fremont Ave
Idaho Falls, ID, 83402
Cristian.Rabiti@inl.gov

ABSTRACT

The Nuclear Regulatory Commission (NRC) has considered revision of 10-CFR-50.46C rule [1] to account for burn-up rate effects in future analysis of reactor accident scenarios so that safety margins may *evolve as dynamic limits with reactor operation and reloading. To find these limiting conditions, both cladding oxidation and maximum temperature must be cast as functions of fuel exposure. To run a plant model through a long operational transient to fuel reload is computationally intensive, and this must be repeated for each reload until the time of the accident scenario. Moreover for probabilistic risk assessment, this must be done for many different fuel reload patterns.*

To perform such new analyses in a reasonable amount of computational time with good accuracy, Idaho National Laboratory (INL) has developed new multi-physics tools by combining existing codes and adding new capabilities. The PHISICS toolkit [2,3] for neutronic and reactor physics is coupled with the RELAP5-3D [4] for the Loss Of Coolant Accident (LOCA) analysis and RAVEN [5] for the Probabilistic Risk Assessment (PRA) and margin characterization analysis. For RELAP5-3D to process a single sequence of cores in a continuous run required a sequence of restarting input decks, each with different neutronics or thermal-hydraulic flow region and culminating in an accident scenario. A new multi-deck input processing capability was developed and verified for this analysis.

The combined RAVEN/PHISICS/RELAP5-3D tool is used to analyze a typical Pressurized Water Reactor (PWR).

INTRODUCTION

Because the nuclear power industry continually improves its designs, safety equipment, processes, and analysis methods, the Nuclear Regulatory Commission (NRC) is considering a revision of the requirements in 10 CFR 50.46C rule, focused on the operation of the Emergency Core Coolant System (ECCS) in Loss Of Coolant Accident (LOCA) scenarios [1]. New analysis strategies will be required to account for the effects of fuel burn-up rate. The maximum temperature and oxidation of the cladding must be recast as functions of the fuel exposure in order to find the limiting conditions of the reactor, with its different design and different reloading patterns.

This revision requires the development of new tools and capabilities to calculate the dynamic phenomena of the multi-physics system to the required accuracy in a reasonable amount of time. To perform such analysis, a rigorous Probabilistic Risk Assessment (PRA) strategy must be employed.

The PRA tool of choice for this analysis at INL is the Reactor Analysis and Virtual-control ENvironment (RAVEN) [5], a generic software framework that performs parametric and probabilistic analysis based on the response of complex system codes. Through its Application Programming Interface (API), RAVEN can communicate with any system code that inputs all the parameters that must be perturbed through files or python interfaces. Currently, RAVEN is coupled to several simulation codes, including RELAP5-3D.

RELAP5-3D [4] is the latest in the RELAP code series of system safety analysis codes developed at INL for modeling transients and accidents in nuclear power plants including advanced reactor designs. Known for its fully integrated, multi-dimensional thermal-hydraulic and kinetic modeling capability, RELAP5-3D capabilities also include modeling moving systems [6] and those with coolants such as molten salts, liquid metals, and supercritical fluids [1]. It also has the ability to couple trough Parallel Virtual Machine (PVM) with other codes [7, 8], such as Computational Fluid Dynamics (CFD), Instrumentation and Control (I&C) and neutronics codes, to solve more complex problems.

RELAP5-3D couples directly with PHISICS for the analysis requirements of the new NRC regulatory consideration of evolving core conditions. The PHISICS code toolkit [2, 3] continues to be developed at INL to provide state of the art analysis tools to nuclear engineers. It implements many choices of algorithms and meshing schemes for optimizing accuracy needs on available computational resources. Currently the PHISICS package contains the following analysis tools:

- INSTANT a nodal and semi-structured transport core solver,
- MRTAU, a depletion module,
- TimeIntegrator, a time-dependent solver,
- MIXER, a cross section interpolation and manipulation framework,
- CRITICALITY, a criticality search module,
- SHUFFLE, a fuel management and shuffling tool.

The tools are developed as independent modules in a pluggable fashion to simplify maintenance and development. To reduce run time, PHISICS can run in parallel on multi-core workstations and high-performance computing systems.

PHISICS is integrated into RELAP5-3D [9] as a set of subroutines that communicate through a Fortran 95 module whose interface subroutines translate physical quantities into the native form of the receiving code. RELAP5-3D sends thermal hydraulic data to PHISICS and receives fission and decay heat power distributions back. It is thus possible for RELAP5-3D to drive an accurate dynamic analysis, switching between steady state, quasi-equilibrium, and time-dependent calculations according to user input.

The RAVEN PRA code runs the PHISICS/RELAP5-3D coupled code for a single set of parameters on an individual computational thread of a cluster supercomputer. It does this for many parameter sets simultaneously, collects the data from the threads then analyzes the data. To operate in this manner requires RELAP5-3D to run restarts of input models, with possible renodalizations of the flow region, without coming to a halt. The new capability to perform restarts in a multi-deck input file was therefore created.

CORE DESIGN

The reference plant chosen for this project is a typical Westinghouse 4-loop Pressurized Water Reactor (PWR). The detailed model is based on a Benchmark for Evaluation And Validation of Reactor Simulations (BEAVRS) [10], having real plant data for assessing the accuracy of reactor physics simulation tools for the first 2 operational cycles. In Fig. 1 and Table 1, the radial core layout and the plant key parameters are shown respectively.

The calculation is performed using homogenized cross sections for each assembly, leading to the identification of 29 different cross section sets for the fuel region and 1 for the radial reflector, composed of the baffle, water between the baffle and the barrel, the barrel and the thermal shield.

For PHISICS/RELAP5-3D, the coupling calculation between the physics is performed through a feedback exchange as shown in Fig. 2. In the upper box, an initial core configuration provides a power distribution to RELAP5-3D, whose native neutronics calculation is bypassed. RELAP5-3D calculates the Thermal-Hydraulics (TH) field and feeds it back to MIXER to calculate cross-sections and INSTANT to recalculate power. The iteration continues until the flow field reaches steady state or a maximum time is reached. The power distribution and temperatures are fed to the depletion calculation of the lower box where the core is burned with a constant temperature field until the fluxes and isotope densities from MRTAU converge and are sent to the upper box. This describes one iteration. Iterations continue until the maximum iterations are reached or the boron concentration (automatically adjusted by the PHISICS code) falls below 5 ppm. Then a new cycle is automatically initiated.

The cross sections sets have been tabulated with respect to several field parameters. For the scope of this work, an *N*-Dimensional grid of 108 tabulation points has been selected, where *N* is number of fuel assemblies.

RELAP5-3D MODELS

The first 10 cycles are used to compute the exposure history of the assemblies but are not an active part of the LOCA simulation, so the TH model contains only the reactor core (without primary and secondary system). For this reason, the primary system is modeled only considering the upper and lower plenum of the core, as shown in Fig. 3. To achieve the greatest accuracy for the determination of the initial conditions in the 11th cycle, the first ten cycles are simulated using one core channel per fuel assembly (193 in total). The radial reflector is modeled as a bypass channel (6% of the mass flow).

The new approach for the analysis of LOCA scenarios requires a detailed burn-up calculation, which strongly impacts the cladding oxidation phenomena. In order to reduce the time of calculation all the power is remapped from 193 assemblies to 6 channels. The model also contains the four loops and the secondary sides of the full PWR plant model [11, 12]. The 6 channels represent:

- 3 different batches (Fresh Fuel, once-burned, twice-burned),
- 3 pins, in the above zones, with the highest peaking factors.

This change in the RELAP5-3D model is accomplished through restart input and represents stage three in each thread shown in Fig. 4. Three input decks are run in succession in a single thread, the 193-channel base deck from Fig. 3, the “Maneuver” restart deck with changes in time step and control rod adjustments to follow prescribed power, and the 6-channel restart deck with renodalization of Fig 4. To run on a single thread, the code cannot cease execution when the processing of one deck ends and the restart begins. The ability to run a deck and its restart without stopping execution is a new capability created to enable this analysis.

RELAP5-3D MULTI-CASE AND MULTI-DECK PROCESSING

RELAP5-3D input processing allows the user to run multiple decks or multiple cases from a single input file to process a sequence of input models.

Multi-case input processing allows the code to run several *related* input models in sequence. However, all runs begin with the same initial conditions from the base case, except where replacement cards modify them. This makes multi-case unsuitable for proceeding from one cycle to the next. Moreover, the new NRC rule requires PHISICS parameters to change, not those of RELAP5-3D.

Multi-deck input processing allows the code to run several *possibly unrelated* input models in sequence. An input file may have several input decks that each end with a "." terminator card. After the first deck is run, processing continues by flushing memory and reading the next input deck from scratch. Additional input decks may occur after the second deck. However, the capability to restart a previous run in a multi-deck file did not exist.

Two modifications enabled the capability in RELAP5-3D to restart a file without cessation of processing in RELAP5-3D. The restart file had to be repositioned at its beginning. The first record written by the restart process must overwrite the record from which the restart data was read. Otherwise, two restart records with the same timestamp exist and cause many issues for the sub-sequential deck, the third in the required sequence for analyzing the new NRC rule.

The new multi-deck restart feature was verified to guarantee it would function correctly for studying the new NRC rule. This is required because when the code runs two input decks without stopping in between, data initialization, file closure, memory deallocation, pointer nullification, and a host of other issues could prevent the code from producing the same answers as if the multiple cases were run separately. This is particularly important when array sizes change during the renodalizing restart that occurs in going from the second to third deck in the analysis.

RELAP5-3D already possesses an extremely accurate verification process for testing base input models and restart runs [13], capable of verifying calculations to 32 decimal places [14]. Recently, the process was extended to test both multi-case and multi-deck runs [15] by automatically separating the internal input cases or decks into separate input decks, running the new decks individually and comparing the resulting verification files to those of the originals. Multi-deck restart testing was incorporated into the verification test suite by creating test input. The testing verified that the multi-deck restart runs produced the same calculations to 32 decimal places as did the standalone runs. With the implementation of the mutli-deck capability verified, it is guaranteed to function correctly for studying the new NRC rule.

MULTI-CYCLE ANALYSIS

In order to assess the compliance of the existing power plants to the new NRC rule, the LOCA accident scenario needs to be initiated in equilibrium cycle conditions, something reached at all nuclear power plants operating in the United States nowadays. Hence, the reactor evolution needs to be followed for several operational cycles, until reaching the reference equilibrium one. The “equilibrium cycle” is generally reached after several reloadings (~18-20). In this study, it is assumed that the equilibrium cycle is reached after the 10th reloading. Figs. 5, 6, and 7 show sample loading patterns after the first, second, third, and later cycles.

The BEAVERS benchmark provides data for the first 2 cycles only (1 reloading pattern). For cycles 3 through 11, new reloading patterns have been constructed. The

BEAVERS reloading is a “high-leakage/low-energy” pattern. The goal here is to perform analysis on a modern reloading pattern; the first developed 4 cycle patterns represent a gradual migration from “high-leakage/low-energy” to “low-leakage/high-energy” reloading patterns. The sub-sequential patterns represent the reference final “low-leakage/high-energy” patterns. All the batch enrichments have been computed in order to reach, at the equilibrium, a cycle length of 18 months.

LOCA ANALYSIS

Fig. 8 shows examples of the assembly-wise radial peaking factors for the Beginning Of Cycle (BOC), Middle Of Cycle (MOC), and End Of Cycle (EOC) at the 10th cycle. Figs. 9, 10, and 11 show the detailed fuel exposure (burn-up) for the same points in time.

At these three points in time, different burn-up levels have been used as initial boundary conditions to analyze the machinery for performing 3 examples of Large Break Loss Of Coolant Accident (LBLOCA) analysis with RELAP5-3D.

This is due to the fact that the LOCA scenarios for the assessment of the safety margins are generally performed considering the reactor immediately after a maneuver that can initiate, for example, a Xenon transient. As already mentioned, for the scope of this work, the maneuver that has been considered is a load-following operation of the reactor.

Figs. 12 and 13 show the results of the analysis. As it can be inferred in Fig. 8 the core status at BOC, MOC and EOC does not determine challenging conditions for the LOCA analysis.

PRA STRATEGY

In order to assess the compliance of the operating nuclear power plants to the new rule, a rigorous PRA is carried out. The new safety margins are related to the cladding oxidation ratio as function of the burn-up level reached by the assemblies when the LOCA scenario is initiated. This means that the limits cannot be seen as static thresholds but must be considered in a dynamic environment, since they evolve during the operation of the reactor.

Another aspect that must be considered in such analyses is the presence of several uncertainties associated with the key parameters of the plant that, depending on their value, can lead to completely different accident scenarios.

From a practical point of view, the goal of the PRA analysis of LOCA events can be summarized as follows:

- Computation of the probability of exceeding the proposed 50.46c safety margins for cladding oxidation,
- Sensitivity analysis on the uncertainty parameters that can influence the LOCA scenario and sub-sequential ranking,
- Identification of the uncertainty parameters' margins through the research of the reliability (or limit) surface.

In order to assess the probability of exceeding the burn-up dependent limit, some sampling of the parameters affected by uncertainties is needed. This kind of analysis is characterized by high level of complexity, including: the computation time of the simulation codes, high dimensionality, cause the uncertainty parameters to take in consideration, and a high discontinuity created by the presence of safety systems that can suddenly start operating. The approach that is going to be used (currently) to perform such analysis is based on the well-known Monte Carlo technique.

The uncertain parameters that will be considered for the analysis are:

- Reactor decay heat power multiplier
- Accumulator pressure multiplier
- Accumulator liquid volume
- Accumulator temperature
- Sub-cooled multiplier for critical flow
- Two-phase multiplier for critical flow
- Superheated vapor multiplier for critical flow
- Fuel thermal conductivity multiplier
- Average temperature
- Film boiling heat transfer coefficient multiplier.

FINAL REMARKS

As near future PRA strategy, in order to overcome the computation burden of the Monte Carlo method, a Hybrid Dynamic Event Tree (HDET) methodology [16, 17] will be used.

The exploration of the system response using the Monte-Carlo (and, in the future the HDET) will ultimately lead to the knowledge of several possible outcomes of the

LOCA accident scenario, in terms of Peak Cladding Temperature (PCT) and corresponding burn-up and oxidation, with their corresponding probability. A post-processing function, built within RAVEN, will allow combining this information to assess what is the final probability to exceed the new limits.

After this preliminary analysis is completed it will be possible to perform sub-sequential investigation where the computation of the sensitivity coefficient will allow to establish what are the most relevant uncertainties effecting the success/failure probability.

Using the RAVEN feature to utilize artificial intelligence accelerated search of reliability surface, it will be possible to use the HDET methodology to determine region of the input space that either leads to a positive/negative final outcome of the LOCA accident.

The newly verified RELAP5-3D multi-case and multi-deck restart capabilities have many applications. Multi-case change data may contain input that modifies the model of the previous input case such as changing tables, switching solvers, and adding, deleting, or modifying hydrodynamic components. A multi-case deck can run multiple perturbations of the original input deck, testing many or every value of the input parameter for a new code feature. It provides for parameter studies wherein one or more values in the initial model can be varied, the model rerun from initial conditions, and the output saved for later analysis. An entire study can be archived in a single file. Modifications to the base model of the file guarantee the same change occurs in all the varied test cases of the study, correctly and automatically.

Multi-deck processing has application beyond the study presented here. For example, a large plot files that is too large to email can be stripped to a manageable size by a second deck. On a multiprocessor, a collection of input models can be grouped to optimize runtime or by resources required. For a model that must run to steady state before initiating a transient, a second deck can restart from the first.

ACKNOWLEDGMENTS

This work was supported by the U.S. Department of Energy (DOE), Assistant Secretary for the Office of Nuclear Energy, under DOE Idaho Operations Office con- tract DE-AC07-05ID14517. The authors of this paper would like to thank Dr. Hongbin Zhang, Paul D Bayless, Dr. Haihua Zhao for performing the LOCA Analysis and for providing us ECR and PCT results.

NOMENCLATURE

API	Application Programming Interface
BEAVRS	Benchmark for Evaluation And Validation of Reactor Simulations
BOC	Beginning Of Cycle
CFD	Computational Fluid Dynamics
CFR	Code of Federal Regulations
CRITICALITY	criticality search module
ECCS	Emergency Core Coolant System
ECR	Equivalent Cladding Reacted
EOC	End Of Cycle
HDET	Hybrid Dynamic Event Tree
I&C	Instrumentation and Control
INL	Idaho National Laboratory
INSTANT	Intelligent Nodal and Semi-structured Treatment for Advanced Neutron Transport
LBLOCA	Large Break Loss Of Coolant Accident
LOCA	Loss Of Coolant Accident
MIXER	cross-section interpolation and manipulation framework
MOC	Middle Of Cycle
MRTAU	Multi-Reactor Transmutation Analysis Utility
N	Number of fuel assemblies
NRC	Nuclear Regulatory Commission
PCT	Peak Clad Temperature
ppm	parts per million
PHISICS	Parallel Highly Innovative Simulation INL Code System
PRA	Probabilistic Risk Assessment
PVM	Parallel Virtual Machine
PWR	Pressurized Water Reactor

RAVEN	Risk Analysis and Virtual-control ENvironment
RELAP5-3D	Reactor Excursion and Leak Analysis Program – Three Dimensional
SHUFFLE	fuel management and shuffling tool
TH	Thermal-Hydraulics
TimeIntegrator	time-dependent solver
t_{LOCA}	LOCA time during the maneuver
t_M	Maneuver time
x	parameters affecting LOCA

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TABLES AND FIGURES

Table 1 – Key plant parameters

No. Fuel assemblies	193
Loading Pattern	w/o U-235
Region 1	1.61 %
Region 2	2.40 %
Region 3	3.10%
Control Rod	Ag-80%, In-15%,Cd-5%
Burnable Absorber	Borosilicate Glass, 12.5 w/o B_2O_3
Power	3411 MW_{th}
Operating Pressure	15.51 MPa
Isothermal Coolant Temperature	564.8 K

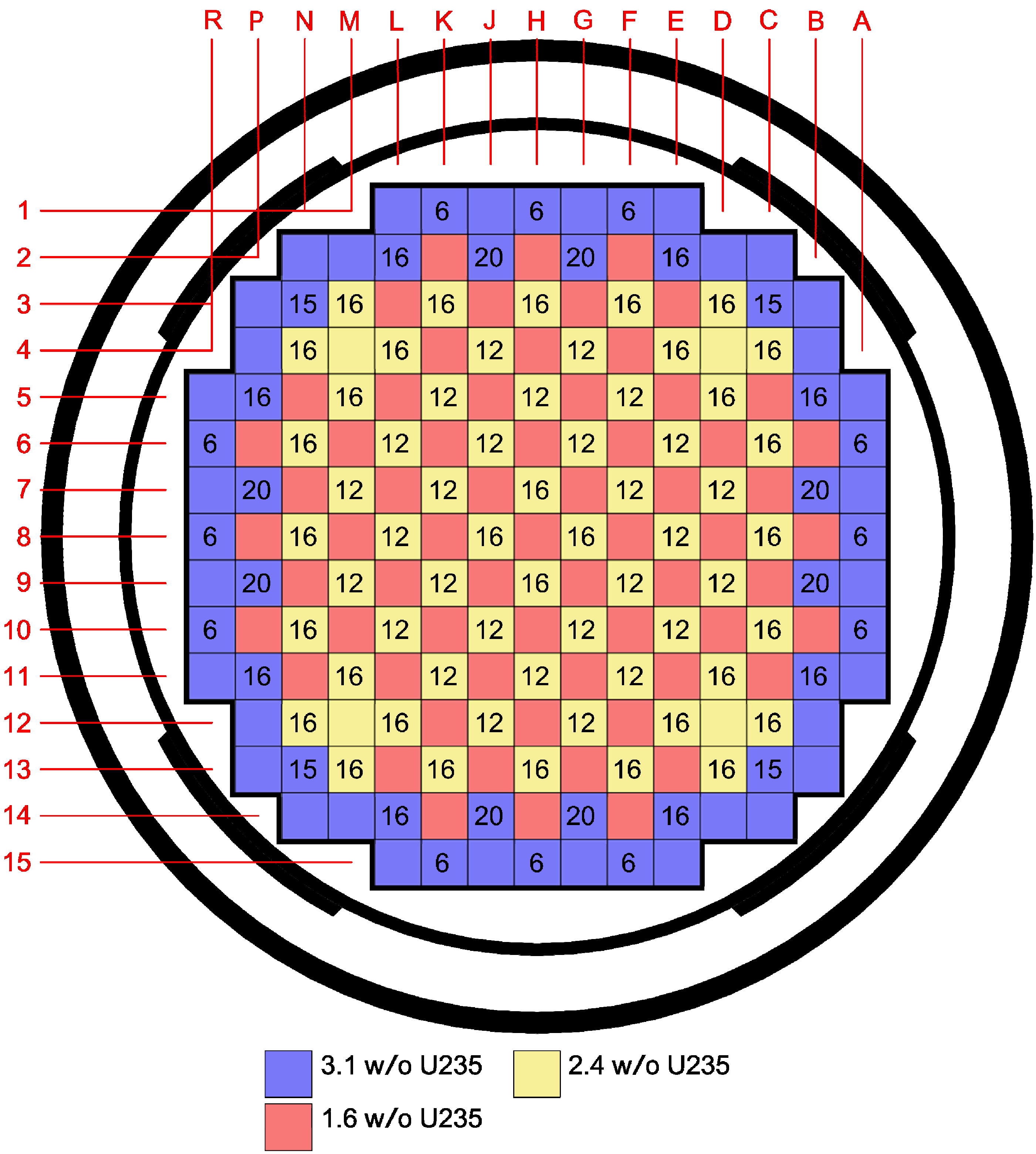


Figure 1. Reactor core layout

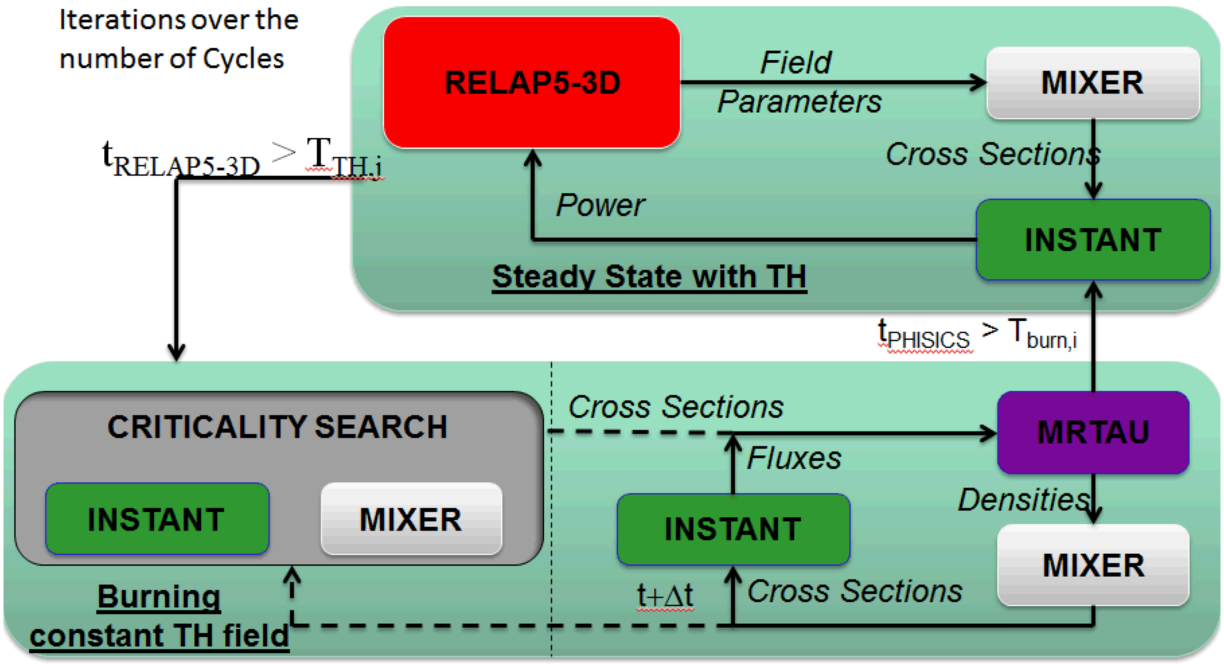


Figure 2. Depletion time evolution coupled with RELAP5-3D

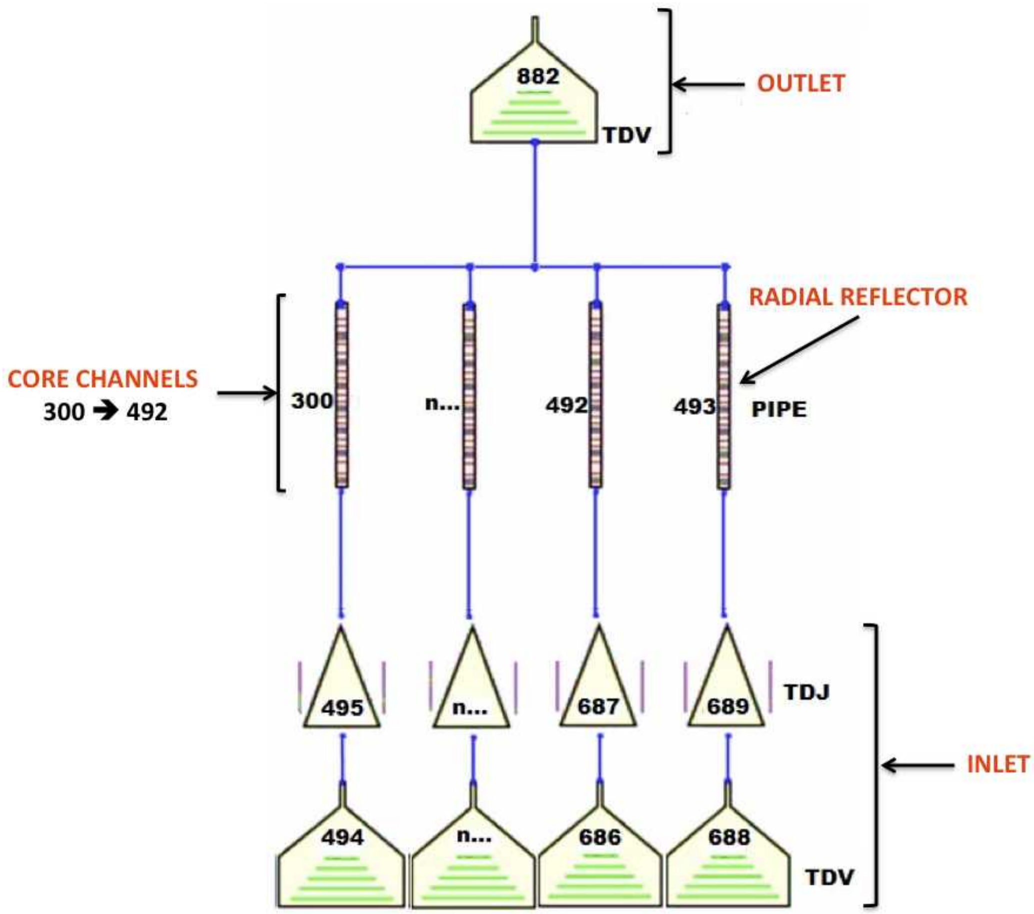


Figure 3. Reactor core RELAP5-3D nodalization

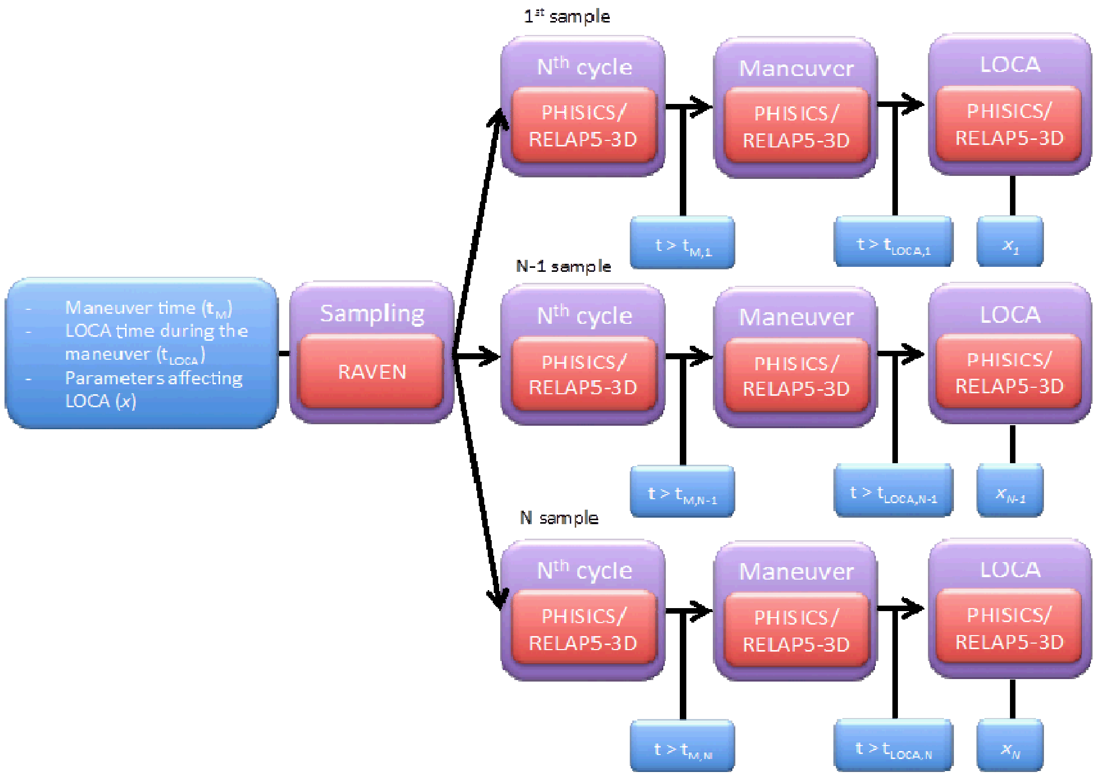


Figure 4. PRA strategy for analyzing the accident scenario from equilibrium core

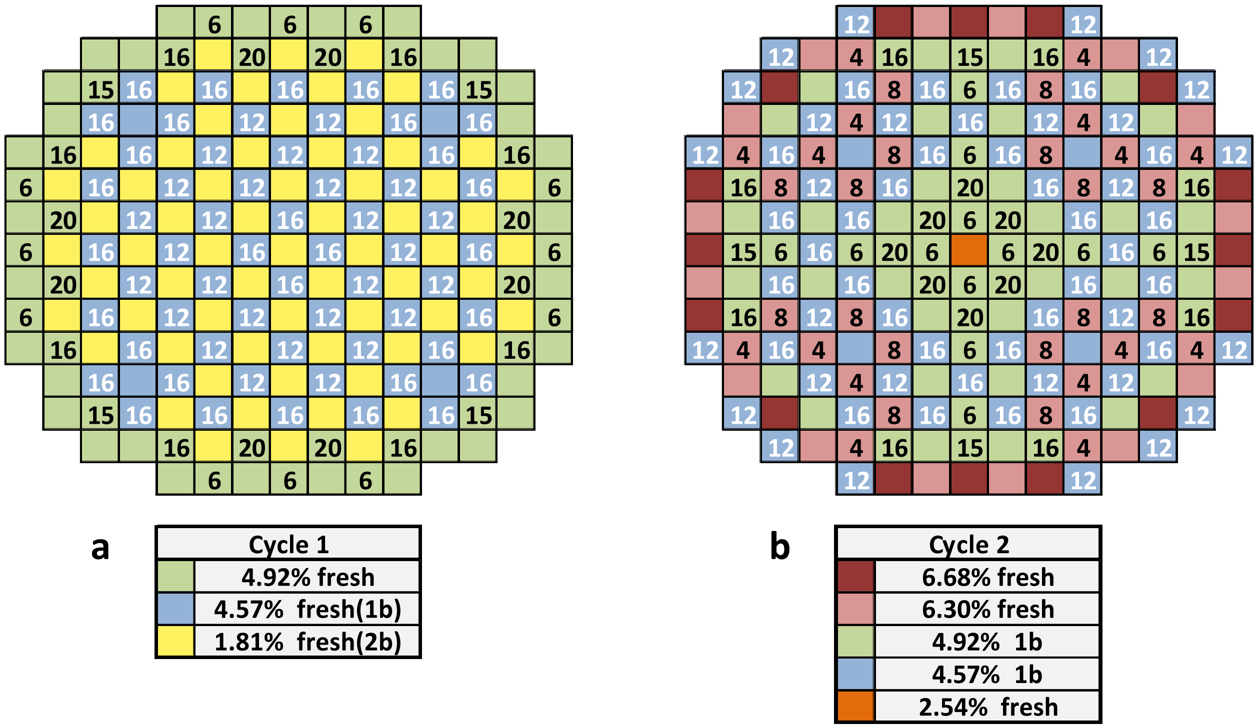


Figure 5. a) 1st Cycle and b) 2nd Cycle Reloading Patterns.

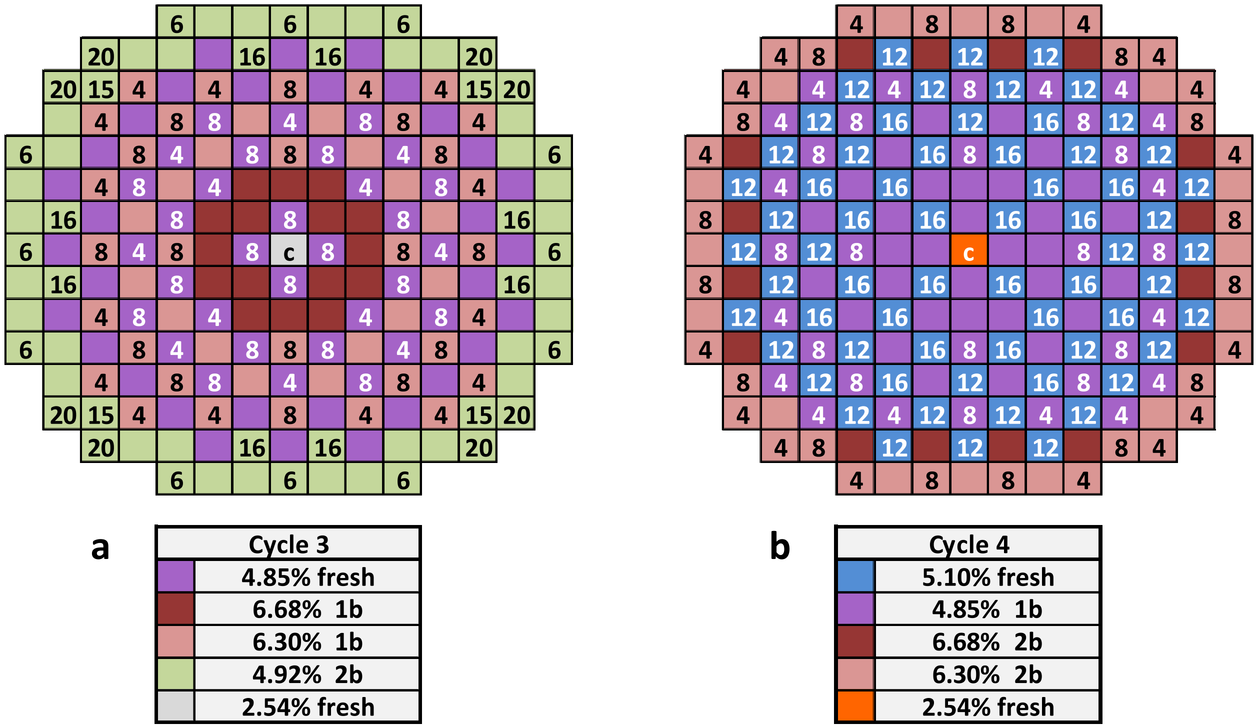


Figure 6. a) 3rd Cycle and b) 4th Cycle Reloading Patterns.

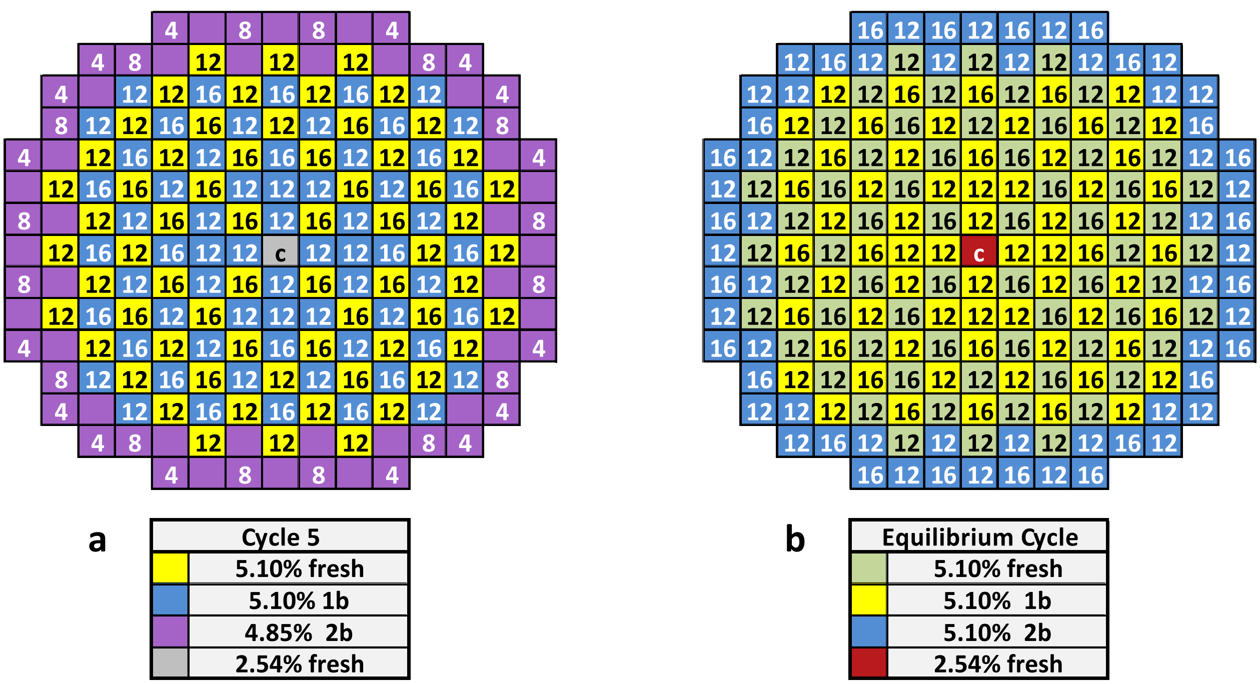
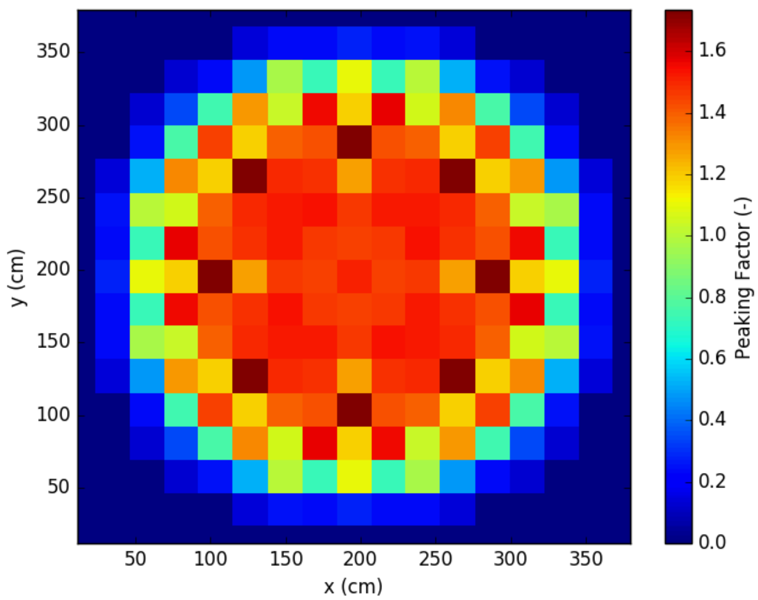
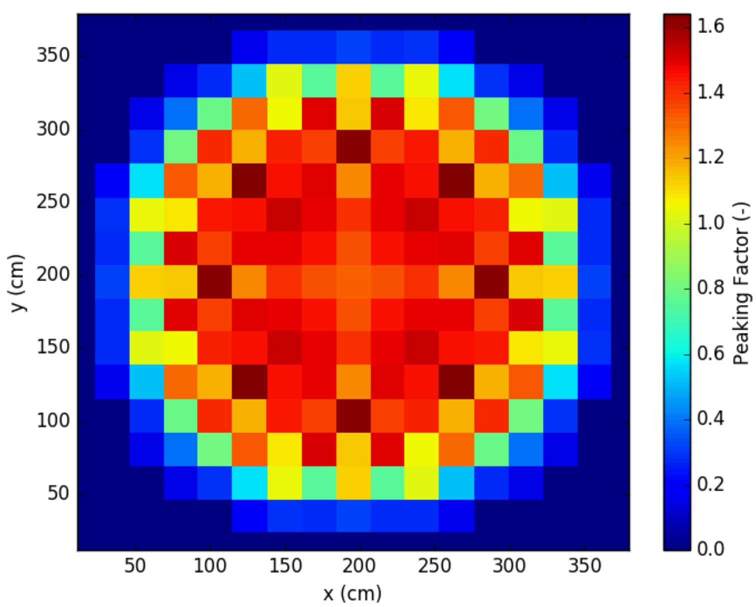


Figure 7. a) 5th Cycle and b) Nth Cycle Reloading Patterns.


y (cm)
x (cm)
Peaking Factor (-)
350
300
250
200
150
100
50
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6


y (cm)
x (cm)
Peaking Factor (-)
350
300
250
200
150
100
50
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6

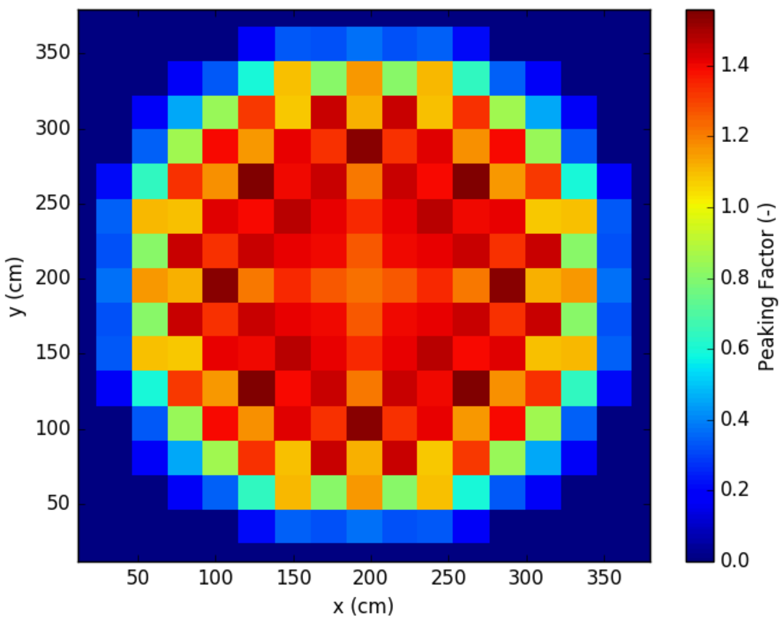


Figure 8. Assembly Peaking Factor for BOC (top), MOC and EOC

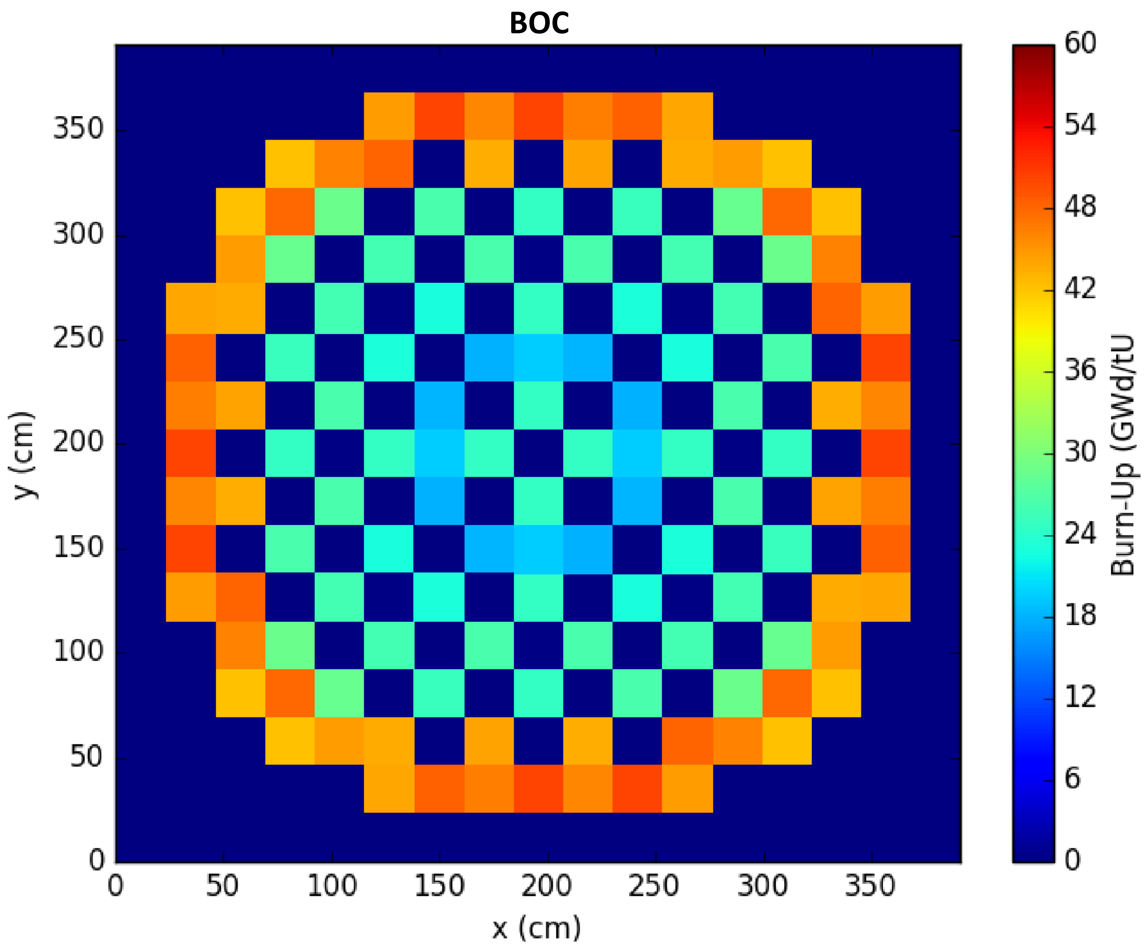


Figure 9. Burnup at Begin of Cycle.

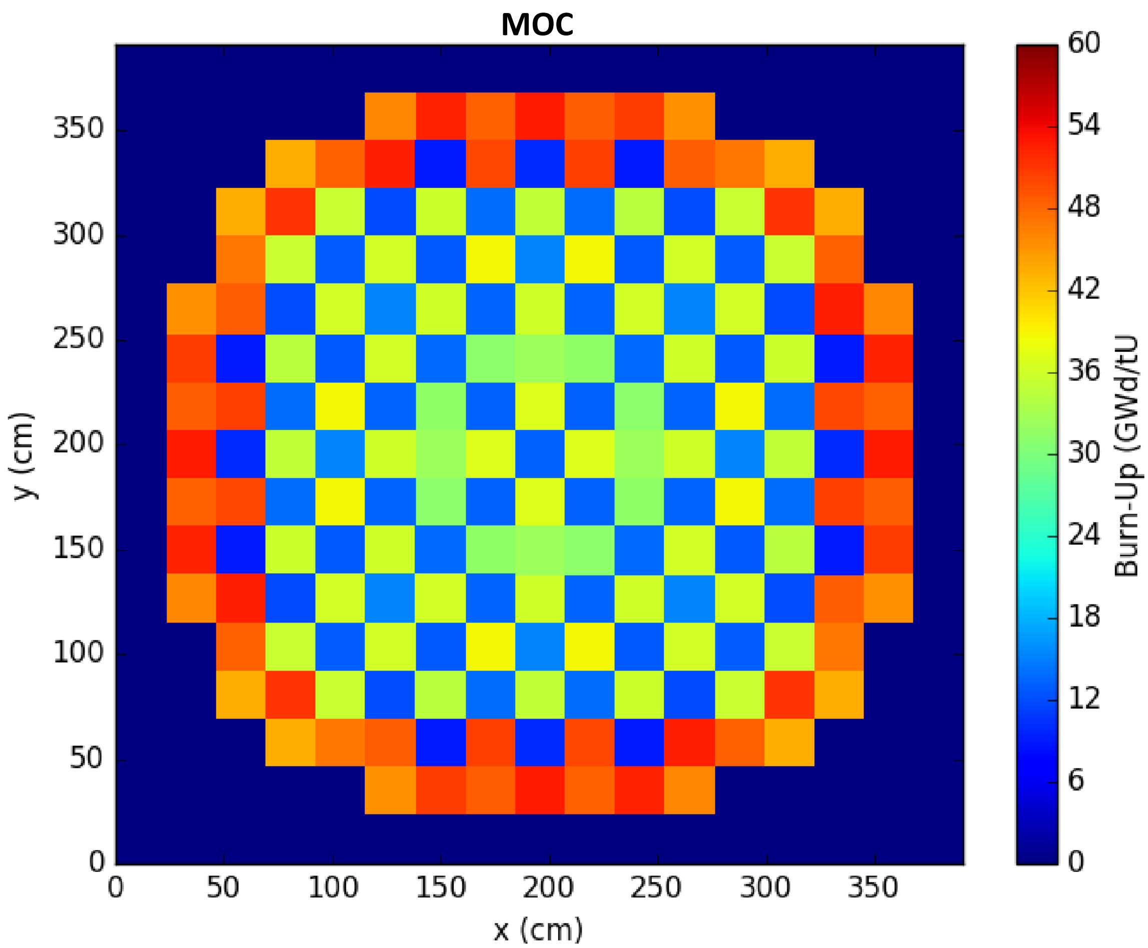


Figure 10. Burnup at Middle of Cycle.

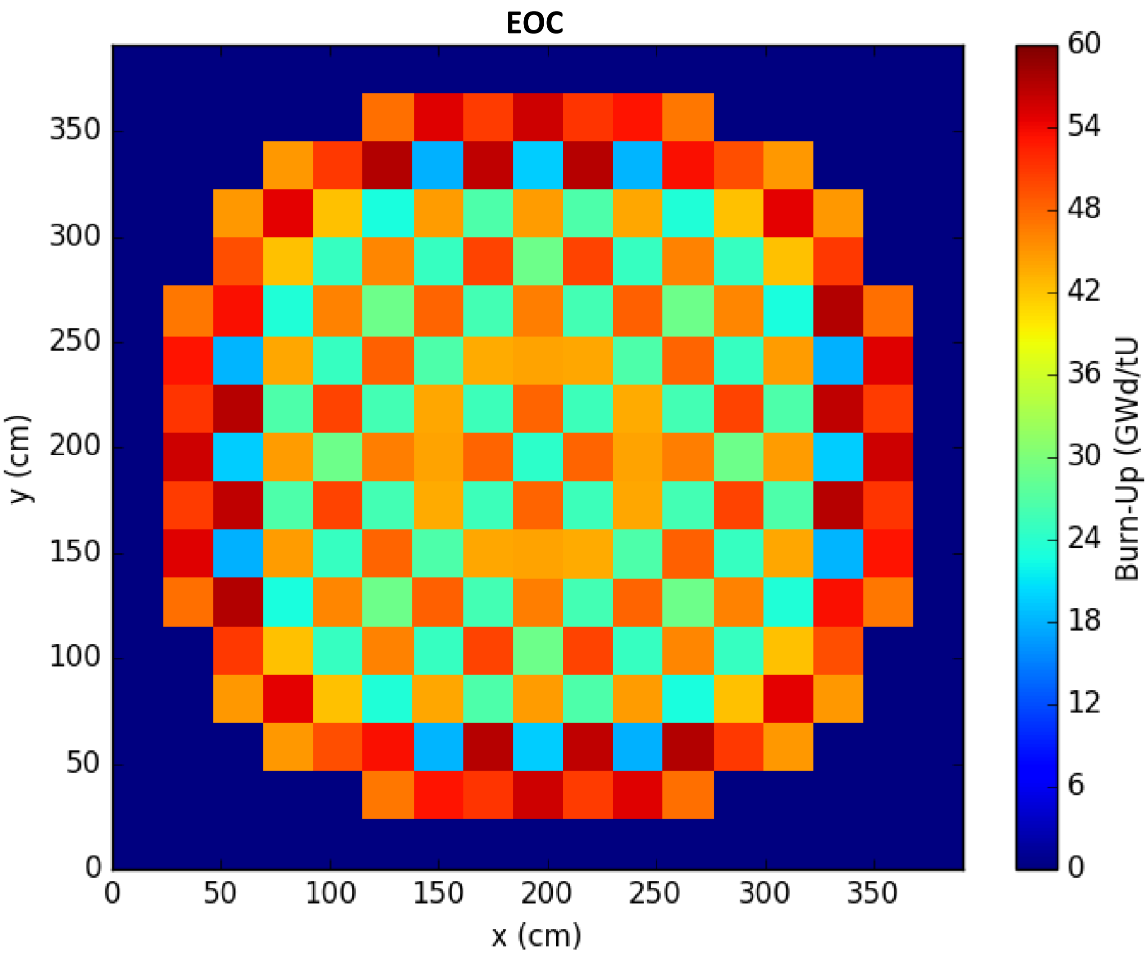


Figure 11. Burnup at End Of Cycle.

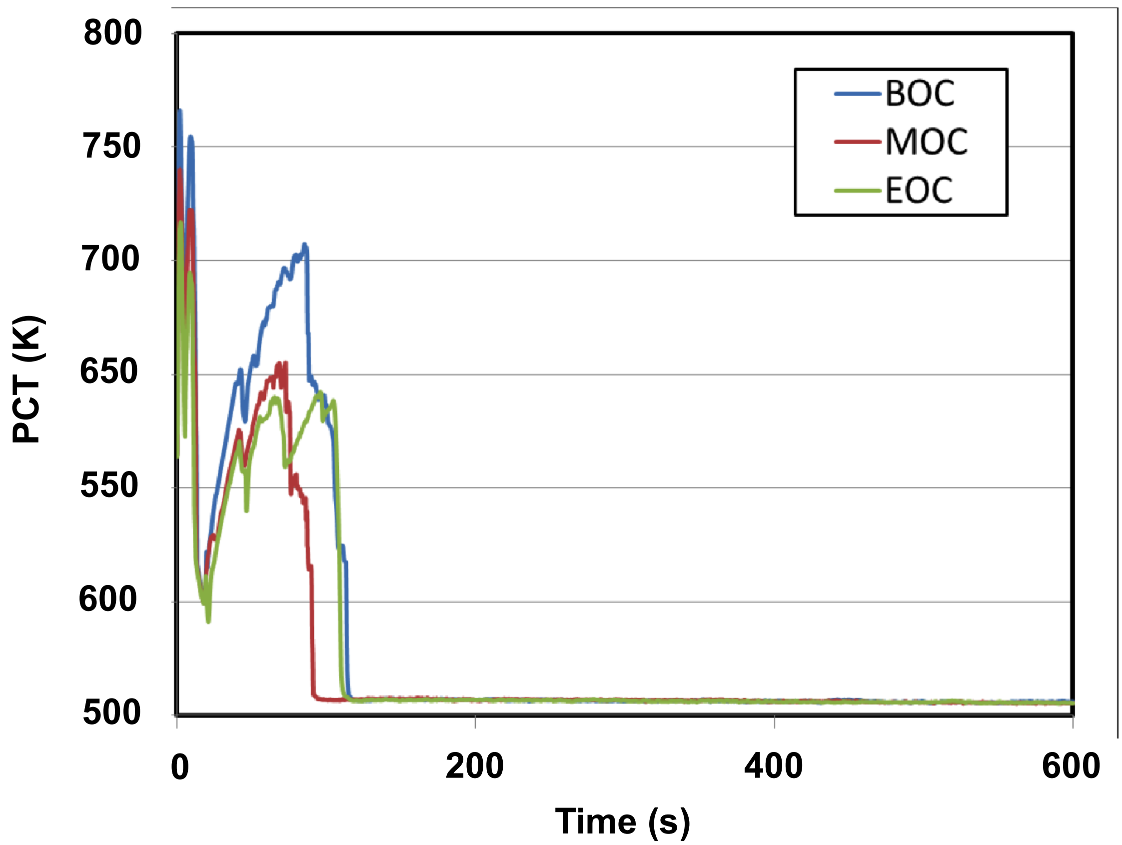


Figure 12. Peak clad temperature during the LBLOCA scenario initiated at BOC, MOC and EOC [9].

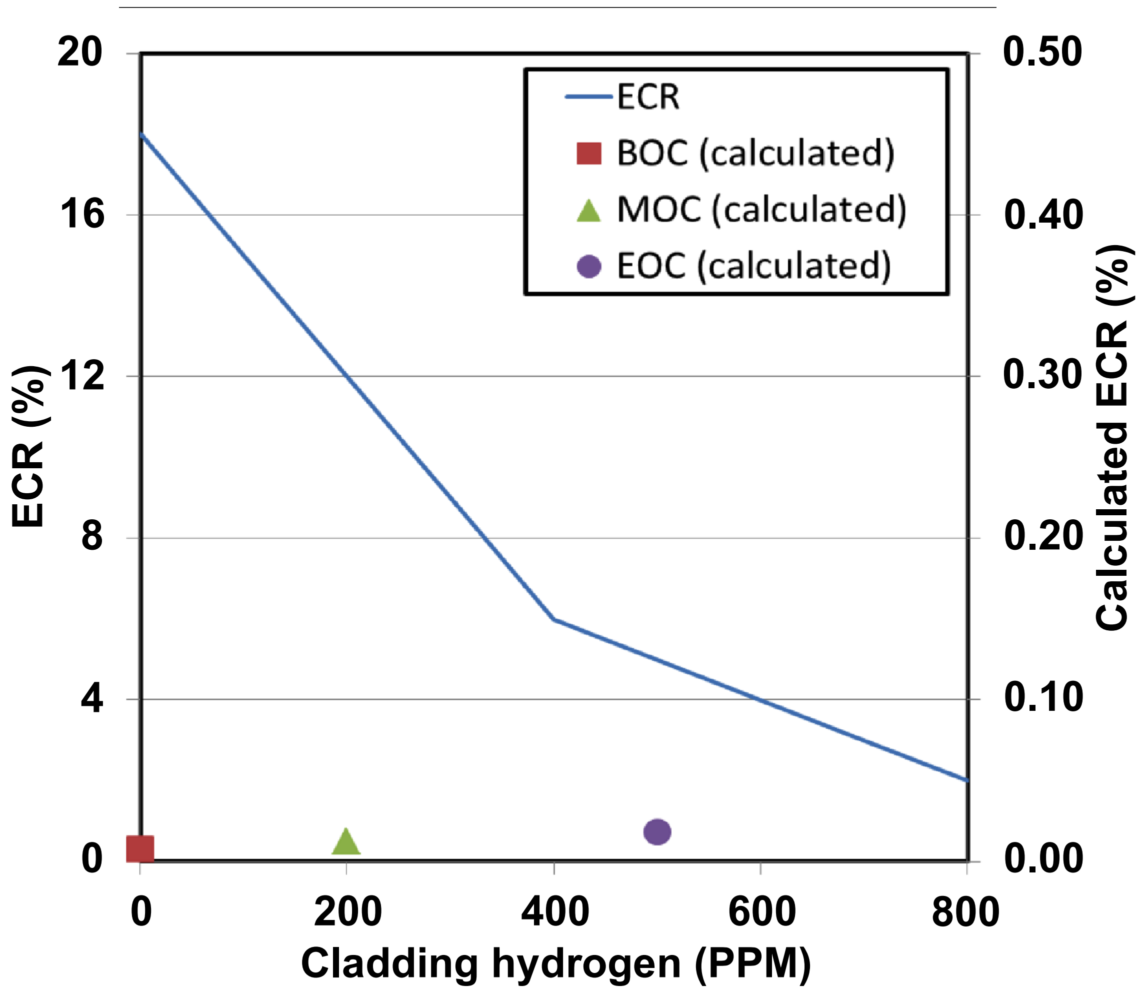


Figure 13. Maximum local oxidation rate during the LBLOCA scenario initiated at BOC, MOC and EOC [9].