FEASIBILITY ASSESSMENT OF ADOPTING THE ADDER COMPUTER CODE FOR THE MIT RESEARCH REACTOR FUEL MANAGEMENT

By

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ABSTRACT

The Massachusetts Institute of Technology Reactor (MITR) is a 6 MW research reactor currently operating with highly enriched uranium (HEU) plate-type fuel. Fuel management calculations for this reactor are performed using MCODE, which allows for the coupling of a neutron transport code and a depletion code. As part of the low-enriched uranium (LEU) fuel conversion program, the Advanced Dimensional Depletion for Engineering of Reactors (ADDER) software is being developed at Argonne National Laboratory to provide a more flexible and performant approach to fuel management. This study evaluates the feasibility of transitioning from MCODE to ADDER for MITR fuel management by carrying out a code-to-code comparison.

Analyses for a full MITR cycle (70 days) for a 22-element fresh HEU core and fresh LEU core were completed, and the impact of simplified in-core experiments with various materials was also evaluated. Calculations with mid-cycle restart were performed, in which reactor power was reduced to 100 kW for 7 hours to evaluate Xe-135 poison reactivity effects. The parameters selected for comparison include control blades height, cumulative fission density, integral neutron flux and nuclide inventory (for selected actinides and neutron poisons).

The study showed satisfactory agreement between ADDER and MCODE results, with control blades worth differences within the 200 pcm range that corresponds to ± 100 pcm critical search tolerance, and U-235 mass differences remaining below 0.5 g per fuel element at end of cycle. Differences for other result types remain low enough to show the potential of transitioning to ADDER, with higher differences located near control blades when using the predictor-corrector method for depletion since the codes rely on different algorithmic definitions for predictor-corrector as well as different critical blade search schedules. Closer agreement between results is obtained when switching to the predictor method but still indicates some potential differences in power normalization. The two software also present good agreement on control blades height and Xe-135 core inventory results for mid-cycle restart calculations.

Further study is recommended to assess depletion factors such as neutron flux normalization and predictor-corrector schemes. Before ADDER is implemented for MITR fuel management, future work is required to evaluate good agreement for equilibrium cores with depleted HEU fuel element compositions, and analyze fuel elements shuffling in between cycles.

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1. Introduction

1.1. Nonproliferation & NNSA Material Management and Minimization Program

The first use of nuclear weapons during World War II and the further development of this technology in the context of the Cold War led to the signing of the Treaty on the Non-Proliferation of Nuclear Weapons (NPT) in 1968. This treaty aims at preventing the dissemination of nuclear weapons, some of which require highly enriched uranium (HEU) to release consequential amounts of energy when used. HEU is defined as 20% or higher concentration of ^{235}U in uranium.

In parallel, the U.S. Department of Energy (DOE) launched in 1978 the Reduced Enrichment for Research and Test Reactors (RERTR) Program, which is currently managed by the National Nuclear Security Administration (NNSA). The main objective of the RERTR Program is the "minimization and, to the extent possible, elimination of the use of HEU in civil nuclear applications by working to convert research reactors […] to the use of LEU fuel and targets throughout the world" [1]. Its primary goal therefore consists in the worldwide conversion of HEU reactors, which were not originally targeted by the NPT, to low-enriched uranium (LEU) that cannot be used in nuclear weapons. LEU is defined as uranium with less than 20% concentration of ^{235}U to total uranium.

The NNSA Material Management and Minimization (M^3) Program oversees this conversion mission which encompasses the conversion of these reactors to existing LEU fuels, as well as the development, qualification, and fabrication of new LEU fuels for research reactors that require specific adjustments to maintain their experimental performance and operational characteristics after the conversion [2]. Part of the mission pertains to the conversion of the U.S. High Performance Research Reactors (USHPRR). The USHPRR include the Advanced Test Reactor (ATR) and ATR critical facility at Idaho National Laboratory, the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory, the University of Missouri Research Reactor (MURR), the National Bureau of Standard Reactor (NBSR) and the Massachusetts Institute of Technology Research Reactor (MITR).

1.2. MIT Research Reactor (MITR) Background

The MIT Research Reactor (MITR), located in Cambridge, Massachusetts, is one of the USHPRR that requires a new high-density LEU fuel to be able to reduce ^{235}U concentration while maintaining operational performances that are suitable for conducting research.

1.2.1. MITR-II Design

The original MIT Reactor, MITR-I, was both heavy-water moderated and cooled with an open array of plate-type fuel elements. This core attained criticality in July 1958 and operated at power levels of up to 5 MW_{th} until 1974. Its second and current core design, MITR-II, began operation up to 5 MW_{th} in 1976, and was approved by the U.S. Nuclear Regulatory Commission (NRC) to operate at power upgrade to 6 MW_{th} during the 2010 license renewal [3].

This current design is a heavy-water (D_2O) and graphite reflected, light-water (H_2O) cooled and moderated tank type nuclear reactor (see Figure 1). It utilizes flat, plate-type, finned, aluminum-clad fuel elements with highly enriched uranium (93.15 wt% ^{235}U) [4]. Specifically, the fuel plates are finned in order to increase the surface area available for heat transfer.

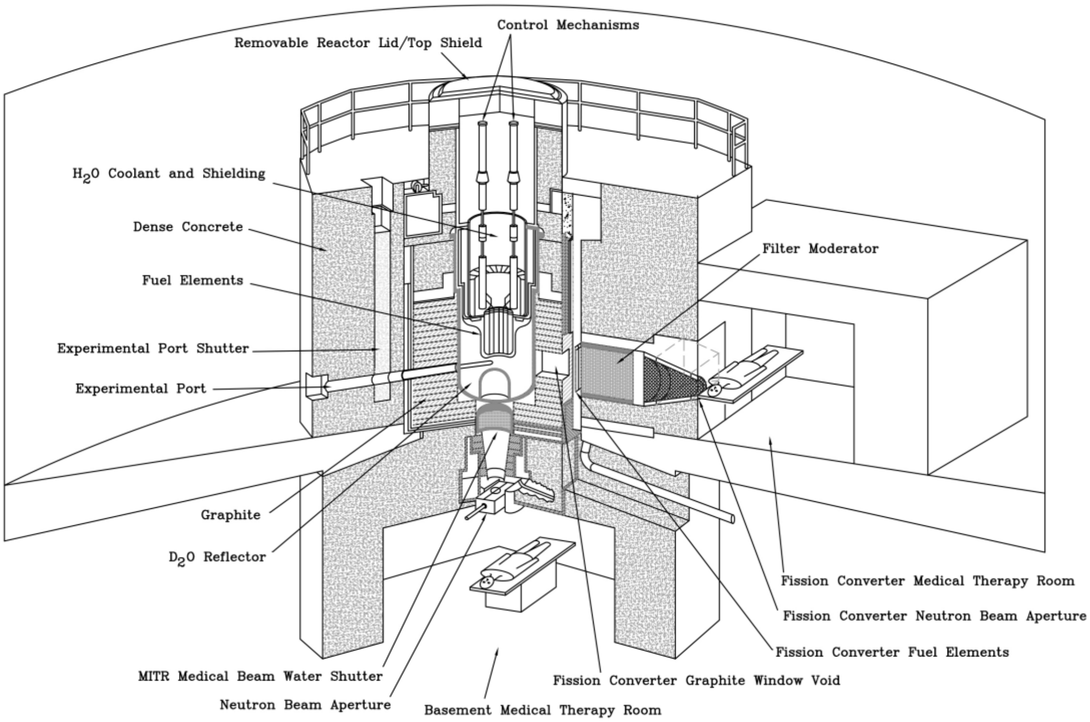


Figure 1: MITR Major Components and Experimental Facilities [3]

The core is made up of 27 rhomboidal fuel positions divided into three rings: A, B, and C (see Figure 2). Twenty-four of these positions contain HEU fuel elements, while the remaining three positions are used for in-core experiments (A-1, A-3, and B-3). The reactor is controlled by using six boron-impregnated stainless steel shim blades and one cadmium regulating rod, located outside of the C-Ring.

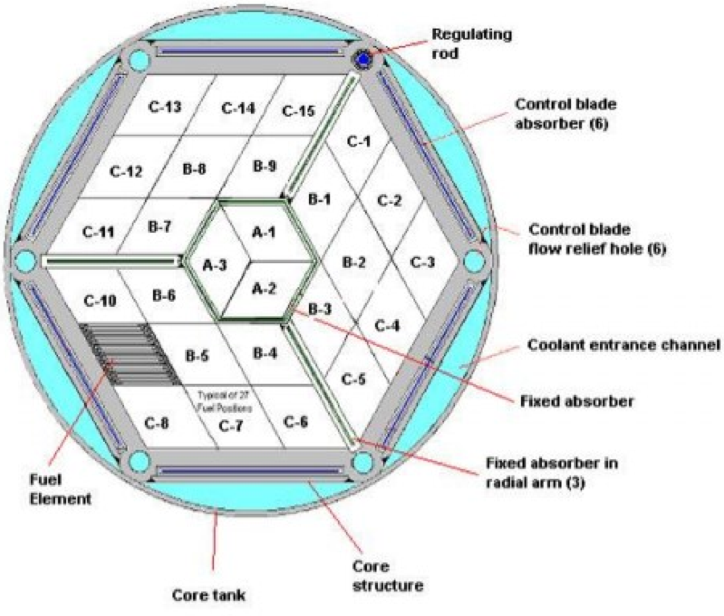


Figure 2: Core Map of MITR [4]

Each fuel element contains 15 identical finned fuel plates composed of HEU in a uranium-aluminum dispersion (UAl_x) which is clad by AA6061 alloy (see Figure 3). The fuel elements are both radially and axially symmetric so that they can be rotated and flipped to equalize the effect of flux peaks on burnup [5]. This feature plays an important role in the MITR fuel management (see 1.2.3).

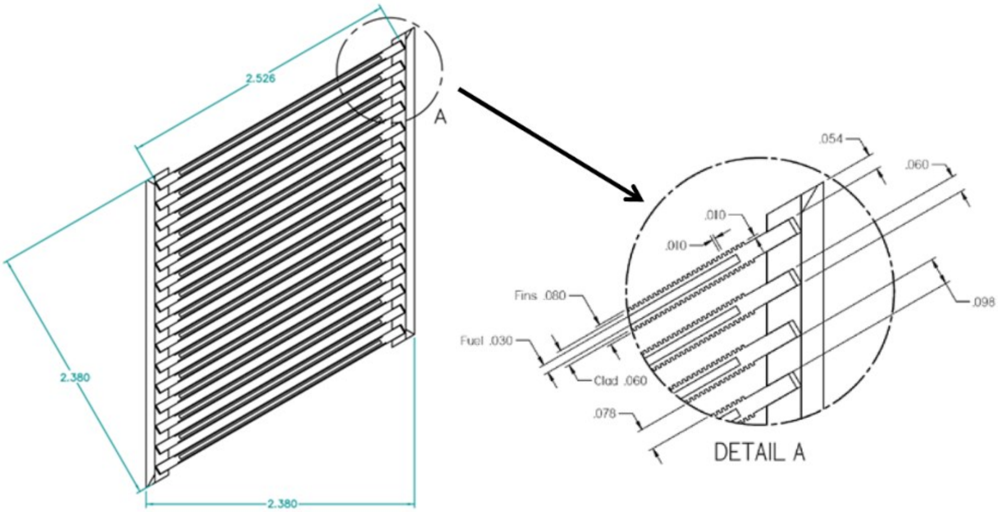


Figure 3: Current MITR HEU Fuel Element (dimensions in inches) [4]

1.2.2. MITR Utilization

The MITR functions both as a center of research and education for MIT departments and other universities. The reactor is also well-utilized by national labs and industry for fuel and materials irradiation tests, as well as a supplier of research radioisotopes for medical and industrial research in the greater Boston area.

Its experimental facilities include a fission converter, horizontal ports to provide neutron beams, irradiation facilities, nuclear instrument penetrations, vertical thimbles in the graphite reflector, in-core facilities, pneumatic tubes, and a thermal neutron beam (see Figure 1), as well as a fuel storage room. Partially depleted fuel elements can also be temporarily stored in the wet storage ring, at the bottom of the core shroud (29 positions). The core design was chosen to maximize the thermal neutron flux in the reflector regions where the experimental beam ports are located.

Given the flexible fuel loading of the MITR-II, in-core sample facilities may occupy one to three in-core fuel element positions (A-1, A-3, and B-3). These facilities have many diverse uses such as a facility for material corrosion and cracking and other material studies under light water conditions, as well as irradiation of fissile materials to evaluate new types of reactor fuel and fuel capsule designs [3].

Materials relevant to the research that is conducted at the MIT Nuclear Reactor Laboratory (NRL) include pressurized water, nuclear-grade graphite, high-temperature molten salt (FliBe), titanium, and cover gas such as helium.

1.2.3. MITR Fuel Management

1.2.3.1. Fuel Management Calculations

MITR fuel management is highly dependent on the reactor core configuration and fuel element depletion history as well as the in-core experiments that can be inserted or removed. It relies on the capability of shuffling fuel elements between different positions in the core, as well as flipping or rotating them. The presence of the shim blades in the higher portion of the core during the reactor operation causes the flux distribution to peak at the bottom. As such, fuel elements are more depleted at the bottom. Flipping the elements is hence very important to achieve a more uniform end of life fuel element burnup.

Detailed neutronic simulations are required to ensure that every new core configuration meets the neutronics safety criteria (cf. 1.2.3.2) and has sufficient excess reactivity to maintain the chain reaction until the end of a fuel cycle. These simulations are coupled with depletion calculations to model the evolution of the fuel elements isotopic composition over time. A typical fuel cycle lasts 70 days, which is representative of the quarterly operating cycle of the MITR (10 weeks of operation / 3 weeks of outage).

Critical blades height searches are also carried out at relevant timesteps to track and adjust the shim blades position so that criticality is maintained throughout the fuel cycle. During such searches, all six shim blades are moved as a group (i.e., shim bank) with the same height [6]. The shim bank height at EOC is one indicator of the excess reactivity of a core configuration: a typical value is 18 inches (45.72 cm) at the end of equilibrium cycles, which represents a 3-inch margin from the 21-inch (53.34 cm) full-out position (see Figure 4) [7].

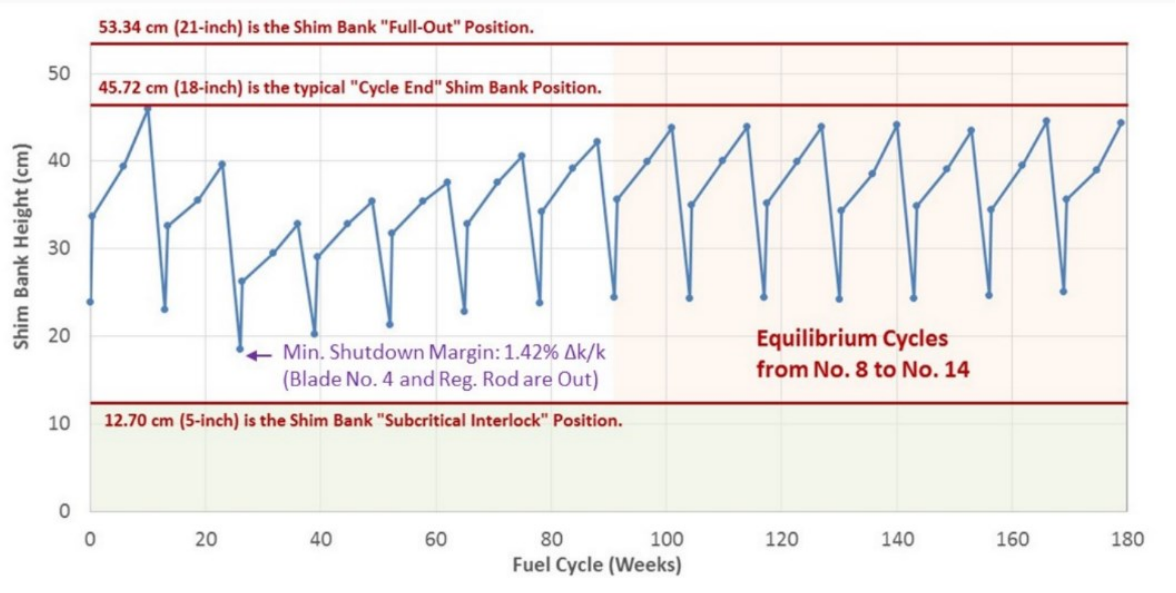


Figure 4: Shim bank movement during transition and equilibrium fuel cycles for LEU cores (computed with MCODE) [7]

These calculations are currently carried out for the MITR with MCODE (cf. 2.3.1.1), an interface program that combines the continuous-energy Monte Carlo code MCNP (cf. 2.1) and the depletion code ORIGEN2 (cf. 2.2) [8].

As part of the Material Management and Minimization (M^3) Program, a new interface code Advanced Dimensional Depletion for Engineering of Reactors (ADDER) is being developed by

Argonne National Laboratory (Argonne) in order to accurately model the USHPRR cores before, during and after their LEU conversion (cf. 2.3.2). This new code supports more complex geometries and fuel management patterns, which can be found in research reactors due to the complexity of their fuel, the presence of in-core experiments and the constraints on their operation and fuel management cycle [9].

1.2.3.2. Neutronics Safety Criteria

One of the primary neutronics criteria used by MITR is the Shut Down Margin (SDM), defined by the NRC as the "instantaneous amount of reactivity by which a reactor is subcritical or would be subcritical from its present condition assuming all full-length rod cluster assemblies (shutdown and control) are fully inserted except for the single rod cluster assembly of highest reactivity worth that is assumed to be fully withdrawn" [10]. The requirement for SDM is such that a given core configuration can be safely made subcritical when accounting for any possible reactivity additions during accident scenarios. The SDM is calculated using the following formula:

$$SDM = \frac{1.000 - k_{\mathrm{lim}}}{k_{lim}} \times 100\% \left[\% \, {}^{\Delta k}/_{k}\right]$$

where k_{lim} is the k_{eff} for a condition in which all the control blades are fully inserted except for the one with highest reactivity worth.

The limiting condition for the MITR is all control blades fully inserted except for the most limiting blade and the regulating rod fully drawn out, for an initially cold (10˚C) and Xenon-free core configuration with all movable and non-secured experimental samples in their most reactive state. For the MITR HEU core, the minimum SDM established as a neutronics safety criterion is 1% ${}^{\Delta k}/_{k}$, meaning the k_{eff} of any evaluated case must be less than 0.99 when the previously described limiting condition is applied [5].

Moreover, a maximum fission density limit of 1.8×10^{21} fissions/cm^3 must be respected in all HEU fuel elements [11].

Finally, the radial power peaking factor F_r must not exceed 2.0 for the studied core as this value was utilized in the calculation of HEU core safety limits [11].

Any new MITR HEU core configuration must be evaluated to meet the previously described neutronics safety criteria. Conformity to such criteria is assessed by carrying out relevant neutronic calculations as part of the MITR fuel management described in 1.2.3.1.

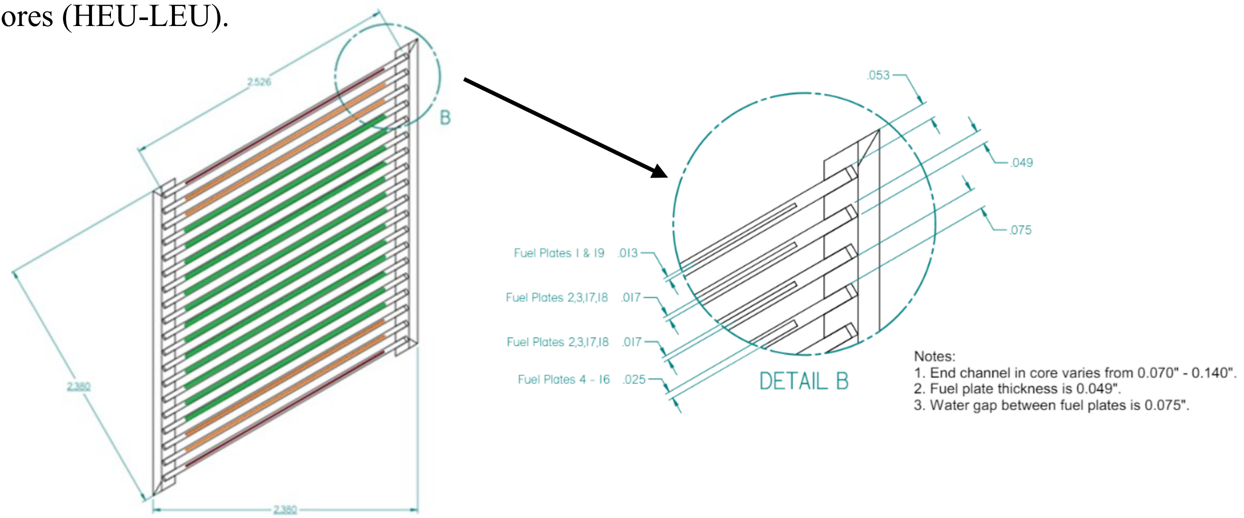
1.3. MITR Conversion to Low Enrichment Uranium (LEU) Fuel

1.3.1. LEU Fuel Element Design

The MITR conversion to LEU requires a modification of the HEU fuel elements described in Figure 3. The proposed MITR LEU fuel elements have the same exterior dimensions as the HEU elements, as well as the same cladding material (AA6061 alloy). The fuel core is an alloy of uranium and molybdenum (U-10Mo) to increase the total uranium density, and the fuel plates in an element have different fuel and cladding thicknesses. The longitudinal fins have been removed to simplify fuel fabrication.

The LEU element contains 19 plates, divided in three different types based on their fuel core thickness: F-type has full-size fuel core thickness and is arranged in the inner part of the element (plates #4 to #15), Y-type has intermediate fuel core thickness (plates #2, #3, #16 and #17) and T-type has thin fuel core thickness and is located in the outer positions of the element (plates #1 and #19). This fuel element design was selected to reduce power peaking in the outer plates, increase total heat transfer area per fuel element and increase the uranium mass per element, which is meant to counterbalance the enrichment decrease and neutron capture of U-238 (see Figure 5).

Table 1 summarizes the difference between MITR HEU and LEU fuel elements [4]. The nominal flow rates are specific to all-HEU and all-LEU cores and may not be applicable to mixed transition cores (HEU-LEU).



Notes:
1. End channel in core varies from 0.070" - 0.140".
2. Fuel plate thickness is 0.049".
3. Water gap between fuel plates is 0.075".

Figure 5: Current Proposed MITR LEU element (dimensions in inches, F-Type in green, Y-Type in orange, T-Type in red) [4]

Table 1: HEU versus LEU Fuel Element Configurations Characteristics Comparison [4]

Parameter	HEU (UAl_x)	LEU (U-10Mo)
Enrichment	93.15 wt%	19.75 wt%
Operating Power	6 MW_{th}	7 MW_{th}
Nominal Flow Rate	2000 gpm	2400 gpm
Plates per Element	15	19
Uranium Density	1.54 gU/cm^3	15.3 gU/cm^3
^{235}U per Element	508 g	968 g
Fuel Thickness	0.76 mm / 30.0 mil	0.64 mm / 25.0 mil (F-Type) 0.43 mm / 17.0 mil (Y-Type) 0.33 mm / 13.0 mil (T-Type)
AA6061 Cladding Thickness	0.38 mm / 15.0 mil	0.28 mm / 11.0 mil (F-Type) 0.38 mm / 15.0 mil (Y-Type) 0.43 mm / 17.0 mil (T-Type)
Zr Interlayer Thickness	-	0.03 mm / 1.0 mil
Plate Thickness	1.52 mm / 60.0 mil	1.24 mm / 49.0 mil

1.3.2. LEU Neutronics Safety Criteria

Similarly to MITR HEU cores, LEU core configurations are required to respect the neutronic safety criteria described in 1.2.3.2.

The LEU shutdown margin is the same as for the HEU case, i.e. 1% $\Delta k / k$ [5].

The maximum LEU fission density depends on the type of plate: it is currently predicted to be 2.0 x 10^{21} fissions/cm^3 for F-Type plates, 2.6 x 10^{21} fissions/cm^3 for Y-Type plates and 3.0 x 10^{21} fissions/cm^3 for T-Type plates [7]. It is expected that a limit on the maximum fission density for the LEU fuel plates would be at or above these values.

The description of the LEU core for neutronic calculations presents an additional level of accuracy (compared to the HEU core) by introducing a radial subdivision of plates into four stripes of equal lengths. This allows for more accurate local results. Consequently, the product of two power peaking factors (radial and lateral) F_rF_s must not exceed 1.677 for interior channels and 1.455 for end channels [5].

Table 2 summarizes the difference between MITR HEU and LEU neutronics safety criteria.

Table 2: HEU versus LEU MITR Neutronics Safety Criteria Comparison

Neutronics Safety Criterion	HEU	LEU
Shutdown Margin	1% $\Delta k / k$	1% $\Delta k / k$
Maximum Fission Density	1.8 x 10^{21} fis/cm^3	2.0 x 10^{21} fis/cm^3 (F-Type) 2.6 x 10^{21} fis/cm^3 (Y-Type) 3.0 x 10^{21} fis/cm^3 (T-Type)
Maximum Power Peaking Factor	$F_r < 2.0$	$F_rF_s < 1.677$ (interior channels) $F_rF_s < 1.455$ (end channels)

1.3.3. HEU to LEU Transition Strategies

One option to transition from the HEU to the LEU configuration for the MITR would be to start off with a LEU core that would contain 22 fresh fuel elements and 5 dummy elements [7]. Some dummy elements and partially depleted HEU elements would then be progressively replaced by fresh LEU elements. Those operations would take place over seven transitional cycles, before reaching an equilibrium fuel cycle state with 24 fuel elements.

Instead of starting off with a fresh LEU core, an alternate MITR conversion from the HEU to the LEU core could be carried out by gradually replacing partially depleted HEU fuel elements with fresh LEU fuel elements [12]. That process would be spread out over 7 mixed HEU-LEU core configurations (MIX-1 – MIX-7), all made up of 24 fuel elements and 3 dummy elements (see Table 3 and Figure 6).

Table 3: Number of LEU versus HEU fuel elements during the mixed core transition cycles [12]

Core Configuration	Number of LEU fuel elements	Number of HEU fuel elements
MIX-0	0	24
MIX-1	3	21
MIX-2	6	18
MIX-3	9	15
MIX-4	12	12
MIX-5	15	9
MIX-6	18	6
MIX-7	21	3
TC-10	24	0

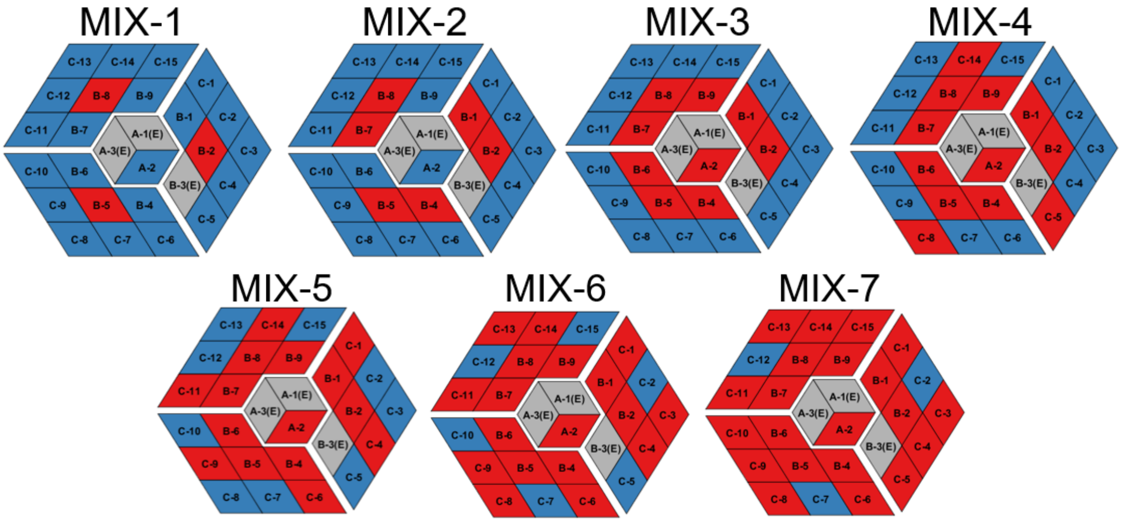


Figure 6: In-core locations occupied by LEU elements (red) and HEU elements (blue) during the mixed core transition cycles. Gray elements indicate in-core experiment positions (A-1, A-3 and B-3) [12]

1.4.Research Objectives and Methodology

1.4.1. Key Steps

The MITR conversion to the new U-10Mo LEU fuel requires modeling of the core with a more suitable tool for fuel management. For instance, modifications are needed for MCODE-FM, the MITR-specific Python wrapper for MCODE (cf. 2.3.1.2), to properly flip LEU fuel elements, which is a drawback for HEU-LEU mixed core or LEU core neutronics analyses. As mentioned in 1.2.3.1, ADDER is being developed by Argonne for the specific analysis of USHPRRs (including MITR) future LEU fuel management. Validating it against MCODE results is therefore crucial before it can be selected as the new MITR fuel management software.

This research project focuses on assessing the feasibility of adopting ADDER as the new MITR fuel management software by completing a code-to-code comparison with MCODE. The selected cases for this comparison need to be representative of the way MCODE is currently used for the MITR fuel management. Moreover, similar options (depletion steps, predictor-corrector method…) will be selected for both MCODE and ADDER calculations, as described in Chapter 2.

The results of the MCODE and ADDER calculations for such cases will be compared to assess the agreement between the software. The following parameters will be analyzed and compared (cf. 3.3):

- k_{eff} values
- Critical shim bank position
- Flux distribution
- Fission density distribution
- Nuclide inventories

Additionally, some software performance parameters, such as critical shim bank height search efficiency, will be documented.

Selected cases for the scope of this study include a fresh HEU core and a fresh LEU core, with several types of simplified in-core experiments representative of the MITR, in order to be able to adopt ADDER as soon as possible.

1.4.2. Fresh HEU Core Study

The modelling of the MITR HEU core can be done following two different paths: considering a fresh HEU core or the current depleted MITR core. Obtaining results with the latter would be of great interest, for they could be compared to current MITR core experimental data, which could be used as part of the validation of ADDER.

However, only the first option will be explored in this work to develop the framework necessary to carry out the code-to-code comparison. The fact that all the plates have the same characteristics in a fresh core facilitates the modelling of this case. Indeed, the only data needed are the MITR core geometry and the fuel elements fabrication specifications (cf. 3.1.1).

1.4.3. Fresh LEU Core Study

After completing the fresh HEU core modelling and study, the main focus of this work is to model the MITR LEU core. Once again, both a fresh LEU core and a depleted LEU core could be analyzed. However, unlike for HEU core configurations, experimental MITR operation data is not available to describe partially depleted LEU fuel elements. The focus of the study will therefore be to model a fresh LEU core.

Such modelling can be carried out using the current MITR geometry, because HEU and LEU fuel elements have the same overall shape. The only difference is the LEU fuel elements geometry (cf. 1.3.1), including different number of plates per element, fuel and cladding thicknesses, and fuel composition (see Table 1).

1.4.4. In-Core Experiments

Because the MITR is used for in-core irradiation of experimental samples, the impact of replacing dummy elements by such samples needs be studied for both HEU and LEU cores, to make sure that these configurations do not cause discrepancies between MCODE and ADDER results.

The experiments to model need to be relevant in light of the research that is conducted at the MIT-NRL (cf. 1.2.2.). The selected main materials include tungsten, graphite and molten salt (FliBe), and the modelling of such experimental samples adopts a simplified geometry, as described in 3.1.3.

1.4.5. Operating Cycle Types

Selected operating cycle characteristics, including cycle length and power level, need to be representative of typical MITR cycles. As described in 1.2.3.1, a typical MITR full cycle is 70-days long at full power, i.e. 6 MW_{th} for the HEU core and 7 MW_{th} for LEU core (cf. Table 1).

Moreover, mid-cycle restarts, which consists of a small period of operation at low power in the middle of a typical full power cycle, need to be studied. Indeed, such power can occur during MITR operation, for instance to insert or remove in-core experiments that only require irradiation during part of the operating cycle. The selected cycle characteristics are described in 3.2.

2. Selected Neutronics Codes

2.1.MCNP5

MCNP5 is a generalized geometry, continuous energy Monte Carlo transport code for neutrons/photons/electrons developed by Los Alamos National Laboratory (LANL) [13]. The selected core configuration is described in a text input file, where surfaces are specified to then build cells, which are filled with user-defined materials. Using tallies, MCNP5 can be used to compute various local quantities in selected cells, such as gamma and neutron flux, reaction rates, etc. Moreover, the k_{eff} can be determined for the studied system, with a standard deviation due to the probabilistic nature of the code (Monte Carlo method).

The main goal of this code is not to perform depletion calculations (even though the latest versions of MCNP include their own depletion solver). It is therefore necessary to interface MCNP5 with a depletion code, such as ORIGEN2 (cf 2.2), in order to compute material composition of core elements including fission products and decay nuclides, so that the reactor state can be determined over an operation cycle. MCODE provides the required interface between MCNP5 and ORIGEN2 (cf. 2.3.1.1).

The version of MCNP5 which is used in this work is MCNP5 v1.60, and the nuclear library used in the MITR modelling is ENDF/B-VII.0 [14].

2.2.ORIGEN2

ORIGEN2 is a one-group depletion and radioactive decay computer code developed by Oak Ridge National Laboratory (ORNL) [15]. It can be used to track the nuclide composition of nuclear fuel over time, whether during irradiation in a reactor core or during decay afterwards. ORIGEN2 can carry out depletion calculations using MCNP-tallied reaction rates, hence the feasibility of interfacing the two codes together to facilitate coupled transport/depletion calculations.

The version of ORIGEN2 which is used in this work is ORIGEN2.2 compiled for thermal reactors. The one-group cross section library used as a starting point is PWRUE.LIB, which represents 4.2 w/o ^{235}U fuel, 3-cycle PWR to achieve 50 MWd/kg burnup, and the decay library used is DECAY.LIB [8].

2.3.Fuel Management Software

2.3.1. Current MITR Fuel Management Software

2.3.1.1. MCODE

The current MITR fuel management neutronics code is MCODE, which is an interface code developed at MIT to couple MCNP (particle transport) and ORIGEN (depletion) to perform burnup calculations for the MITR. MCNP is used to model the reactor and tally the energy-integrated reaction rates in pre-defined spatial burnup zones. These results are passed on to ORIGEN, which carries out depletion calculations to update the material compositions in the MCNP model. MCODE allows to automate successive runs of the two codes, as well as the data transfer in between.

A MCODE input file consists of a MITR MCNP model, followed by selected MCODE options, such as MCNP and ORIGEN executables and libraries path, MCNP tally specification and depletion options (constant flux or power, predictor or predictor-corrector method, timesteps and power levels, number of substeps, and material-specific options: ORIGEN library, volume, neutron absorption fraction threshold).

The version of MCODE which is used in this work is MCODE-2.2 [8], which provides an interface between MCNP5 v1.60 and ORIGEN2.2 (thermal).

a. ORIGEN library update with MCNP-computed data

For material m, nuclide n and reaction type r, reaction rates R_{mnr} and energy-integrated region-averaged flux values Φ_m are provided by MCNP flux tallies (track length estimates), by integrating over energy as follows:

$$\Phi_m = \int \phi_m(E)dE$$

$$R_{mnr} = \int \sigma_{nr}(E)\,\phi_m(E)dE$$

These results allow MCODE to compute microscopic one-group cross sections $\sigma_{mnr} = {}^{R_{mnr}}/_{\Phi_m}$, which are used to update the ORIGEN one-group cross section library.

Moreover, even if the reaction can lead to either a ground state or an excited state nuclide, only the total one-group cross section σ_{tot} is computed by MCNP. In this case, the ORIGEN library is updated with the corresponding one-group cross sections σ_{ex} and σ_{grd} in a way that preserves the branching ratio (BR) that can be found in the selected library (PWRUE.LIB for this work), where $BR = \frac{\sigma_{ex}}{\sigma_{grd}+\sigma_{ex}} = \frac{\sigma_{ex}}{\sigma_{tot}}$ [8].

b. Flux normalization

The MCNP-generated one-group flux values are in units of (number of neutrons) per cm^2 per (fission source neutron) and need to be converted to (number of neutrons) per cm^2 per second. This flux normalization is carried out by multiplying the MCNP-flux by the Flux Normalization Factor (FMF, in fission source neutron per second):

$$FMF = \frac{P \times \nu}{Q_{ave} \times k_{eff}}$$

where P is the user-specified total power of the system (Watts);

ν is the average number of neutrons produced per fission;

Q_{ave} is the average recoverable fission energy released per fission (J/fission);

k_{eff} is the MCNP-computed eigenvalue of the system.

The recoverable fission energy release Q for an individual heavy metal nuclide n (atomic number Z and mass number A) is computed by MCODE as follows:

$$Q_n = 1.29927 \times 10^{-3} Z^2 \sqrt{A} + 33.12$$

Q_{ave} is then obtained by averaging over the different materials m (in the different regions) and nuclides n as follows:

$$Q_{ave} = \frac{\sum_m \sum_{n\in m} Q_n N_{mn} V_m \int \sigma_{n,fis}(E)\phi_m(E)dE}{\sum_m \sum_{n\in m} N_{mn} V_m \int \sigma_{n,fis}(E)\phi_m(E)dE}$$

$\nu = k_{eff}\, {}^{w_{src}}/_{w_{floss}}$ is computed with the following MCNP results: eigenvalue k_{eff}, weight of source neutrons w_{src} and weight loss to fission w_{floss} [8].

c. Nuclide selection process

Typical ORIGEN one-group cross section libraries contain ~1000 nuclides while MCNP is only used to calculate a small subset of important nuclides according to the neutron absorption ranking. This is done due to the excessive MCNP CPU time demand and the unavailability of many neutron cross section libraries.

When updating the material composition in the MCNP model, the inclusion of nuclides is therefore determined by MCODE through the user-specified absorption fraction threshold. All nuclides existing at the beginning of life will always be included, and the remaining nuclides are included in descending order of the neutron absorption ranking until the absorption fraction satisfies the user-specified threshold [8].

d. Predictor-corrector method

In order to produce more accurate results, the user can select a predictor-corrector approach to determine updated material compositions. This method consists in performing two depletion calculations (instead of one). The predictor reaction rates are generated by MCNP with initial material compositions and used to deplete initial materials from beginning to end of timestep to obtain predictor end-of-timestep compositions. These compositions are used to generate the corrector reaction rates with MCNP, which are used to deplete initial materials from beginning to end of timestep and obtain the corrector end-of-timestep compositions. The average between the predictor and corrector end-of-timestep material compositions is selected to update the MCNP model [8].

2.3.1.2. MCODE-FM

A MITR-specific Python wrapper for MCODE was developed to automate fuel management neutronics calculations. This wrapper, MCODE-FM [16], consists of a collection of Python scripts designed to assist with the initial MCODE input creation for a selected MITR core configuration and operating cycle description, as well as with the critical shim blades height search in between depletion time steps.

MCODE-FM was validated against MITR HEU experimental results [17]. Two cases were experimentally carried out at the MITR and modeled in MCODE-FM. The first case consisted of a startup to full power from a Xenon-free state, without any in-core experiment. The reactor operated for 100h at 5.7 MW_{th} before the power was reduced to 10 kW_{th} for 130h, followed by a shutdown. This case allowed for a comparison of Xenon reactivity effects, as well as shim bank heights throughout the different phases. The second case consisted of two irradiations of steel wires in a capsule inserted in position A-3 (5.4 MW_{th} for 32.8 days and 5.7 MW_{th} for 30.5 days). This case allowed for a comparison of reaction rate-based thermal and fast neutron fluxes, which “can be determined by measuring the decay of radioactive activation products of the introduced steel wires” [17]. Both cases showed good agreement between experimental and MCODE-FM results.

e. Input files

MCODE-FM requires 5 input files to run a calculation [16]:

control_input	Description of the MCNP transformations that act on the shim bank, as well as its withdrawal range (0-53.34 cm).
keffsearch.py	Script that carries out the critical shim bank height search by moving the shim bank in the MCNP model.

mcnp.sh	Script that allows for modification of the number of tasks assigned to the calculation, and to perform a criticality search before the MCNP flux calculation for ORIGEN.
mcode_input	Description of the lengths of the cycles and respective reactor powers, as well as the fuel element positions and states (flipped/rotated or not) during the different cycles, the number of plates / axial nodes / lateral nodes for each element, and the isotopic composition of each material filling up a fuel cell at beginning of a cycle.
skeleton_input	MCNP model of the MITR (including shim blades and regulating rod), except for the fuel elements.

MCODE-FM uses the material description in the *mcode_input* file to build the fuel elements and complete the model in the *skeleton_input* file. The MCNP cross section library to use for each isotope is specified in *skeleton_input* for non-fuel materials, and in *mcode_input* for fuel materials. The library used for the MITR is ENDF/B-VII.0 at 293.6K (.70c [18]) for all isotopes (cf 2.1). Moreover, the cycle lengths and reactor powers are used for depletion.

f. Critical shim bank height search

Finally, a critical shim bank height search is carried out by *keffsearch.py*, which moves the blades according to the transformations and range described in *control_input*. The critical shim bank height search adopts the following algorithm to move the shim bank until criticality is reached:

- **First iteration**: a MITR-specific Differential Worth (DW) of 0.0027 .cm^{-1} is hardcoded in the script. The next guess height z_2 is found using the following formula:

$$z_2 = z_1 + \frac{1 - k_1}{DW}$$

where z_1 is the initial shim bank height and k_1 is the eigenvalue when the shim bank is at position z_1.

- **Next iterations:** the differential worth is computed using the results from the two previous calculations:

$$DW = \frac{k_{n-1} - k_{n-2}}{z_{n-1} - z_{n-2}}$$

where z_{n-1} and z_{n-2} are the two previous shim bank heights, and k_{n-1} and k_{n-2} are the eigenvalues when the shim bank is at position z_{n-1} and z_{n-2} respectively.

The next guess height z_n is found using the following formula:

$$z_n = z_{n-1} + \frac{1 - k_{n-1}}{DW}$$

Criticality is reached at step n if $[k_n - \sigma_n, k_n + \sigma_n] \subset [1 - tol, 1 + tol]$, where tol is the tolerance, set at 0.001 (100 pcm) in *keffsearch.py* for this work.

g. Selected options

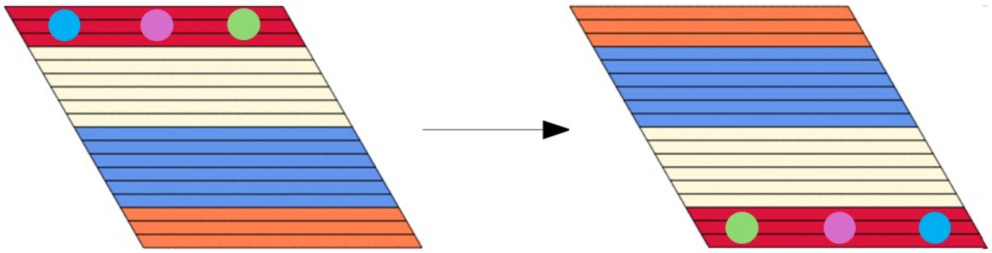
For MITR fuel management calculations, the following MCODE options are automatically selected by MCODE-FM when creating the MCODE input file:

ORIGEN library (for all materials)	PWRUE.LIB (cf 2.2), updated with MCNP-generated one-group cross sections

Neutron absorption fraction threshold	0.999, i.e. 100 pcm (cf. 2.3.1.1)
Depletion normalization	Constant power depletion
Depletion method	Predictor-corrector (cf. 2.3.1.1)
Number of depletion substeps (during one depletion timestep)	20
Depletion timesteps (in between which a critical shim bank height search is performed)	If the cycle is less than 40 days: day 0, day 1, day 3, end of cycle If the cycle is more than 40 days: day 0, day 1, day 3, day 40, end of cycle

Because of the way MCODE-FM handles fuel plates definition and element rotation, it cannot be used to correctly rotate LEU fuel elements in its current state. Indeed, instead of rotating the elements (180-degree turn), MCODE-FM reverses the order of the radial materials, as described in Figure 7. The rotation is therefore correctly carried out if the fuel plates are not subdivided into lateral nodes (MITR HEU core), but this operation is not accurate when lateral segmentation is selected by the user (see Figure 7).

180-degree rotation



Material order inversion (MCODE-FM)

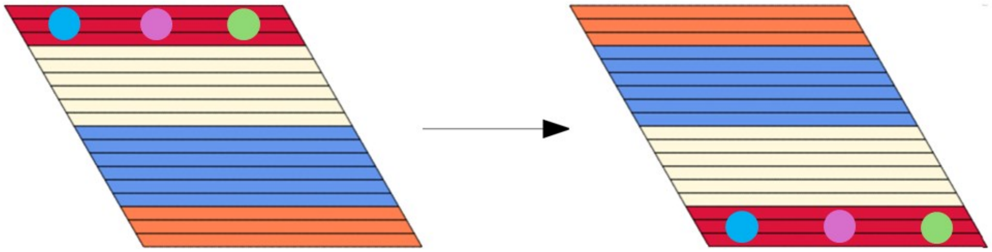


Figure 7: Comparison of a 15-plate element rotation during fuel management (top) and MCODE-FM calculations (bottom) [22]

Lateral segmentation is not used for current MITR HEU calculations but has been selected for MITR LEU analyses (4 equal lateral nodes). This implementation of element rotation in MCODE-FM would therefore need to be modified before it could be used for conversion-related studies and post-conversion fuel management calculations.

2.3.2. ADDER

ADDER is a new fuel management neutronics tool developed at Argonne National Laboratory (Argonne) for reactor design and analysis. Similarly to MCODE, it provides an interface between a transport solver and a depletion solver to carry out cycle-long neutronics studies.

In its current state (v1.0.1), ADDER can use MCNP5 or MCNP6 for transport calculations, and ORIGEN2 or an internal Chebyshev rational approximation method (CRAM) solver for depletion calculations. Its features include the ability to deplete the reactor for a given power history, shuffle fuel in the core and load or remove fuel from the core, and perform criticality searches and stochastic volume computations [9].

The necessity to rotate, flip and shuffle LEU fuel elements for the MITR fuel management justifies the transition from MCODE to ADDER for fuel cycle calculations. Moreover, ADDER provides an improved user experience by reducing the number of required inputs (compared with MCODE-FM), and by presenting the results in a unified HDF5 file (cf. 4.2.1.2). Finally, the maintenance of MCODE over the years is difficult to implement because there is no dedicated technical staff involved in its development and maintenance at MIT. Indeed, this situation increases the complexity of knowledge transfer for the software. On the other hand, ADDER development is managed by Argonne, which will ensure the routine maintenance and verification and validation process through software quality assurance standards and procedures in place at the laboratory. For the aforementioned reasons, ADDER was selected as a potential replacement to MCODE to perform MITR fuel management calculations.

The version of ADDER which is used in this work is ADDER v1.0.1, which provides an interface between MCNP5 v1.60 and ORIGEN2.2 (thermal) [9].

a. ORIGEN library update with MCNP-computed one-group cross sections

Using the same method as MCODE (cf. 2.3.1.1), ADDER can update the ORIGEN one-group cross section library by using MCNP-generated fluxes and reaction rates. This option can be selected by the user in the ADDER input file [9].

b. Flux normalization

ADDER carries out flux normalization from MCNP units to ORIGEN-compatible units using the same method as MCODE (cf 2.3.1.1) [19].

c. Nuclide selection process

At the end of an ORIGEN depletion calculation, ADDER selects the nuclides to keep in the updated MCNP model according to a user-defined neutronics reactivity threshold. For each depleted material m, the reactivity worth ρ_n of each nuclide n is first assessed using the following formulas (the flux is determined from the latest transport calculation):

$$\nu\Sigma_{m,fis}\Phi_m = \sum_{j\in m} N_{jm} \int \nu\sigma_{j,fis}(E)\phi_m(E)dE$$

$$\Sigma_{m,abs}\Phi_m = \sum_{j\in m} N_{jm} \int \sigma_{j,abs}(E)\phi_m(E)dE$$

$$k_{\infty,unperturbed} = \frac{\nu\Sigma_{m,fis}\Phi_m}{\Sigma_{m,abs}\Phi_m}$$

$$k_{\infty,perturbed\ for\ n} = \frac{\nu\Sigma_{m,fis}\Phi_m - N_{nm}\int \nu\sigma_{n,fis}(E)\phi_m(E)dE}{\Sigma_{m,abs}\Phi_m - N_{nm}\int \sigma_{n,abs}(E)\phi_m(E)dE}$$

For a fissionable nuclide, the reactivity worth is:

$$\rho_n = \left|\frac{k_{\infty,unperturbed} - k_{\infty,perturbed\ for\ n}}{k_{\infty,perturbed\ for\ n}}\right|$$

For a non-fissionable nuclide, the reactivity worth is:

$$\rho_n = \frac{N_{nm} \int \sigma_{n,abs}(E)\phi_m(E)dE}{\Sigma_{m,abs}\Phi_m}$$

For a selected material m, once all reactivity worths have been computed, the nuclides are sorted by ascending worth, and the set of isotopes whose total reactivity worth is less than the user-defined neutronics reactivity threshold are filtered out from being included in the updated MCNP model [9].

d. Predictor-corrector method

ADDER allows the user to choose between a predictor or a predictor-corrector method for depletion calculations. The predictor-corrector method implemented in ADDER is based on the Constant Extrapolation/Constant Midpoint (CE/CM) algorithm, where a first step (predictor) consists in depleting materials until the midpoint of the user-selected depletion timestep. The MCNP model is then updated with the midpoint material compositions to compute the midpoint reaction rates, which will be used to carry out depletion between the start and the end of the timestep (corrector) [9].

e. Input files

ADDER requires 2 input files to run a calculation:

adder_input	Description of the user-selected number of tasks assigned to the calculation and ADDER global options that will be applied to all operations, as well as the different operations to apply to the initial model (critical shim bank height search, depletion and power history, fuel element rotation / flip / shuffling).
mcnp_input	MCNP model of the MITR at beginning of cycle.

ADDER uses the MCNP model described in the *mcnp_input* file to sequentially carry out the different operations described in the *adder_input* file. The MCNP model is updated at the end of each operation. The library used for the MITR is ENDF/B-VII.0 at 293.6K (.70c [18]) for all isotopes and all operations (cf. 2.1).

f. Critical shim bank height searches

The critical shim bank height searches carried out by ADDER adopt the following algorithm to move the shim bank until criticality is reached:

- **First iteration**: the Differential Worth (DW) is computed by using the bounds of the user-defined shim bank height range in the *adder_input* file $[z_{low}, z_{upp}] = [12.70, 53.34]$ (cm) for the MITR (from the subcritical interlock position to the full-out position [7]):

$$DW = \frac{k_{upp} - k_{low}}{z_{upp} - z_{low}}$$

where k_{low} and k_{upp} are the eigenvalues when the shim bank is at position z_{low} and z_{upp} respectively. z_{upp} and k_{upp} are replaced by z_{guess} and k_{guess} if the user specifies a shim bank height guess in the ADDER input.

The next guess height z_2 is found using the following formula:

$$z_2 = z_1 + \frac{1 - k_1}{DW}$$

where $z_1 (= z_{upp})$ is the initial shim bank height and $k_1 (= k_{upp})$ is the eigenvalue when the shim bank is at position z_1.

- **Next iterations:** the differential worth is computed using the results from the two previous calculations:

$$DW = \frac{k_{n-1} - k_{n-2}}{z_{n-1} - z_{n-2}}$$

where z_{n-1} and z_{n-2} are the two previous shim bank heights, and k_{n-1} and k_{n-2} are the eigenvalues when the shim bank is at position z_{n-1} and z_{n-2} respectively.

The next guess height z_n is found using the following formula:

$$z_n = z_{n-1} + \frac{1 - k_{n-1}}{DW}$$

The search is considered converged at step n if $[k_n - 2\sigma_n, k_n + 2\sigma_n] \subset [1 - tol, 1 + tol]$, where tol is the tolerance, set at 0.001 (100 pcm) in *adder_input files* for this work.

For each shim bank position guess, ADDER adjusts the number of batches so that the calculations are more precise (but computationally more costly) when the guess gets closer to the target.

g. Selected options

For MITR fuel management calculations, the following ADDER options have been selected in the *adder_input* files:

ORIGEN library (for all materials)	PWRUE.LIB (cf 2.2), updated with MCNP-generated one-group cross sections
Neutron reactivity threshold	0.001, i.e. 100 pcm
Depletion normalization	Constant power depletion
Depletion method	Predictor-corrector (CE/CM)
Number of depletion substeps (during one depletion timestep)	20
Order of operations (to copy MCODE-FM default behavior)	If the cycle is less than 40 days: Critical shim bank height search (day 0) - Depletion for 1 day Critical shim bank height search (day 1) - Depletion for 2 days Critical shim bank height search (day 3) - Depletion until end of cycle Critical shim bank height search (end of cycle) If the cycle is more than 40 days: Critical shim bank height search (day 0) - Depletion for 1 day Critical shim bank height search (day 1) - Depletion for 2 days Critical shim bank height search (day 3) - Depletion for 37 days Critical shim bank height search (day 40) - Depletion until end of cycle Critical shim bank height search (end of cycle)

3. Core Configurations for the Feasibility Assessment

3.1. Fresh Fuel Core Configurations

3.1.1. Fresh HEU Core

3.1.1.1. Fresh HEU Core Configuration

The fresh HEU core configuration selected for this work consists of 22 fresh HEU fuel elements (15 plates, cf. 1.2.3.1), and 5 aluminum dummy elements in positions A-1, A-3, B-3, B-6 and B-9 (see Figure 8). This configuration is similar to the MITR Core II, which was part of the initial startup of the reactor in 1976 [20]. Two dummy elements were added in positions B-6 and B-9 to the typical MITR core configuration (cf. 1.2.1), in order to reduce the excess reactivity of fresh fuel (compared with partially depleted fuel). In the selected configuration, the fuel plates have a parallel orientation for each core zone, as described in Figure 8. Moreover, no element is flipped or rotated during a fuel cycle.

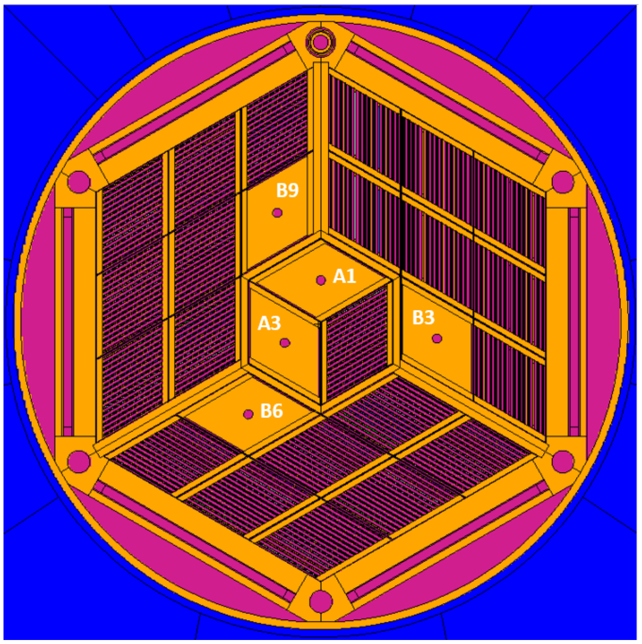


Figure 8: Selected Fresh HEU Core Configuration
(plotted in MCNP5)

3.1.1.2. Fresh HEU Core Modelling

The fresh HEU core configuration described above is modelled in MCNP5 by MCODE-FM. This model was developed by Everett Redmond II, and incrementally edited to increase accuracy and model new types of in-core experiments [21].

The base model of the MITR is described in the *skeleton_input* file. This model contains all components from the MITR, except for fuel elements. Among the modelled MITR components, reactivity control systems include both the shim bank height and the cadmium regulating rod (cf. 1.2.1). The former is used to carry out power level changes (startup / shutdown) and maintain the system critical as fuel elements are being depleted over time, while the latter is used to fine-tune reactivity and correct small perturbations, but its impact is not significant over longer depletion steps. The regulating rod is therefore not taken into account during the critical search algorithm (cf. 2.3.1.2) and modelled at a fixed 2-inch withdrawn position in the *skeleton_input* file.

On the other hand, the shim blades are at the heart of the search algorithm, for they can be moved vertically using transformations 100-101, 200, 300-301, 400-401, 500, and 600-601. These transformations are used by *keffsearch.py* to move the shim bank during a critical shim bank height search without having to redefine surfaces in the MCNP model. The shim bank range is specified at the end of the *control_input* file (0-53.34 cm). If the aforementioned transformations are not in this range in the *skeleton_input* file, an error is raised by MCODE-FM. Moreover, 12 ppm of boron is added in the water (material 1) to fine-tune the shim bank height after comparison with MITR shim bank height logs. Finally, the kcode card to write in the *skeleton_input* file for this work was selected after the analysis described in 4.1.3.

The *mcode_input* file specifies the power history (each new power or element shuffling starts a new "cycle") and the position of each fuel element in the core (see Figure 1.2.1). For each position, the user can write cards followed by the selected option to describe the way MCODE-FM should model each fuel element. Cards are divided in two blocks: the "path" block, which describes the element state in the core (fuel or in-core experiment, position, rotation, flip, shuffling) and the "element" block (axial and lateral segmentation, radial grouping, material description for each fuel node) [22].

Each HEU fuel element is divided into 15 plates and 16 equal axial nodes without lateral striping. The axial segmentation (including axial nodes height) is described in Figure 9. The fuel zones are shown in orange, and the non-fuel zones at the top and bottom of the fuel element are shown in gray and are modelled as two homogeneous cells in the MCNP file.

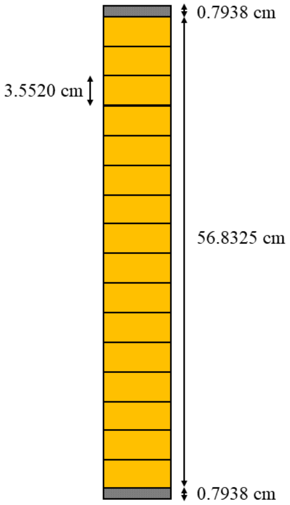


Figure 9: Axial Segmentation of MITR Fuel Elements

MCODE-FM uses the user input in the "element" block to write the relevant surfaces for axial nodes segmentation in the full MCNP model (*mc000i* file in the *tmpdir11* folder) under the name "FUEL SEGMENTATION". Vertical surfaces that define the fuel plates are already written in the *skeleton_input* file (surfaces 71XXX and 72XXX), and do not include fins to simplify the model. When building plates, MCODE-FM sequentially fills the cells with water (blue), cladding (gray), fuel (orange), and cladding, and repeats this pattern as described in Figure 10 to accurately model fuel plates and the in-between water channels.

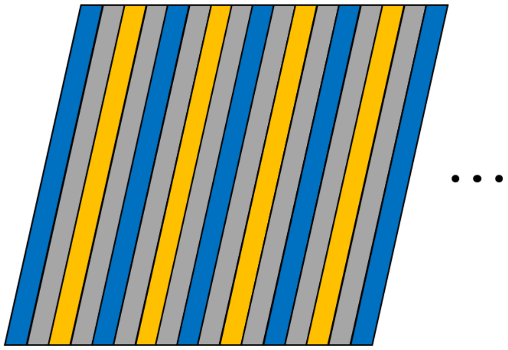


Figure 10: Plates Specification of HEU Fuel Elements

Each HEU fuel cell consequently has the following dimensions and volume:

- Height: 3.5520 cm
- Thickness: 0.0762 cm
- Width: 5.2883 cm
- Volume: 1.4313 cm^3

Moreover, MCODE-FM creates one new universe per defined fuel element in the *mcode_input* file, starting with universe 1, and then fills each core position (cells 101 to 127) with the corresponding universe. MCODE-FM also writes fuel elements cell importances (imp:n=1) and temperatures (tmp=3.2154e-8) in a vertical format, as well as tally materials and flux tallies.

The *mc000i* file created by MCODE-FM as the initial fresh HEU core model is also used as the MCNP input for ADDER calculations, after undergoing a few modifications by using the *MCODE_to_ADDER_conversion.py* script. Indeed, the current version of ADDER does not support vertical format for cell importances and temperatures, requires all materials to have a library specified through the nlib card, and moves the shim blades by modifying surfaces during the critical search (unlike MCODE-FM which modifies transformations). Therefore, the following edits need to be made for the input file to be usable by ADDER:

- Erase MCODE tally materials and MCODE tallies;
- Convert cell importances and temperatures from the vertical format to the horizontal format (cell by cell);
- Add nlib card to all materials;
- Change shim blades transformations to 0.

Finally, the same cards are added at the beginning of all adder_input files, to make sure that only fuel cells are depleted, and that shim blades are correctly moved during critical searches (cf. Appendix A).

3.1.2. Fresh LEU Core

3.1.2.1. Fresh LEU Core Configuration

Similar to the fresh HEU core described above, the fresh LEU core configuration selected for this work consists in 22 fresh LEU fuel elements (19 plates, cf. 1.3.1), and 5 aluminum dummy elements in positions A-1, A-3, B-3, B-6 and B-9 (see Figure 11), as described in [20]. In the selected configuration, the fuel plates have a parallel orientation for each core zone, as described in Figure 9. Moreover, no element is flipped or rotated during a fuel cycle.

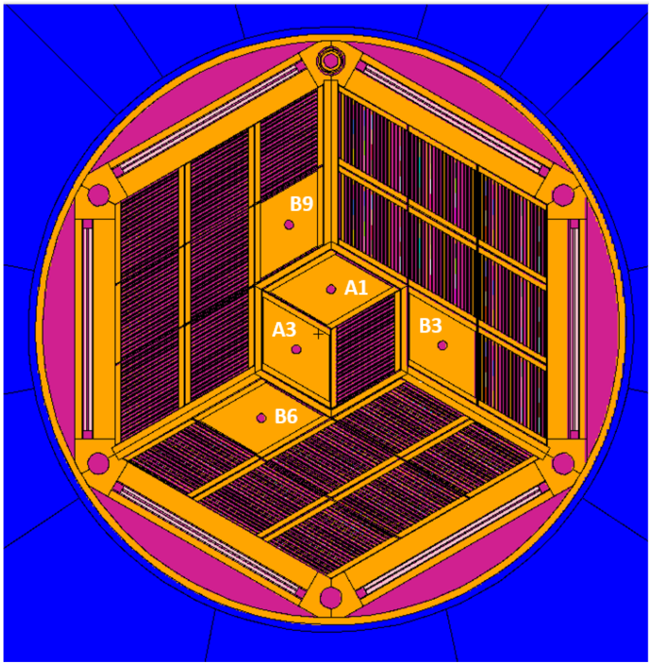


Figure 11: Selected Fresh LEU Core Configuration (plotted in MCNP5)

3.1.2.2. Fresh LEU Core Modelling

The fresh LEU core configuration described above is modelled in MCNP5 by MCODE-FM.

As described in 3.1.1.2, the base model of the MITR is described in the *skeleton_input* file, and the elements specifications are described in the *mcode_input* file. The regulating rod and the shim bank are modelled similarly to the fresh HEU case, but no boron is added in the water (material 1). The kcode card is also selected according to the analysis described in 4.1.3.

Each LEU fuel element is divided into 19 plates (FYT-types, cf. 1.3.1), 16 equal axial nodes and 4 equal lateral nodes to increase the accuracy of results for thermal hydraulics analyses of the LEU core [7]. The axial segmentation is the same as the HEU case, which is described in Figure 9.

MCODE-FM uses the user input in the "element" block to write the relevant surfaces for axial and lateral nodes segmentation in the full MCNP model (*mc000i* file in the *tmpdir11* folder) respectively under the names "FUEL SEGMENTATION" and "LATERAL SEGMENTATION". Vertical surfaces that define the fuel plates are already written in the *skeleton_input* file (surfaces 81XXX and 82XXX). The MCODE-FM script *subs.py* had to be modified to take into account the new number of plates and the new plate surfaces. When building plates, MCODE-FM sequentially fills the cells with water (blue), cladding (gray), fuel (orange), and cladding, and repeats this pattern as described in Figure 12 to accurately model fuel plates (divided in four equal lateral nodes) and the in-between water channels.

LEU fuel cells consequently have the following dimensions and volumes:

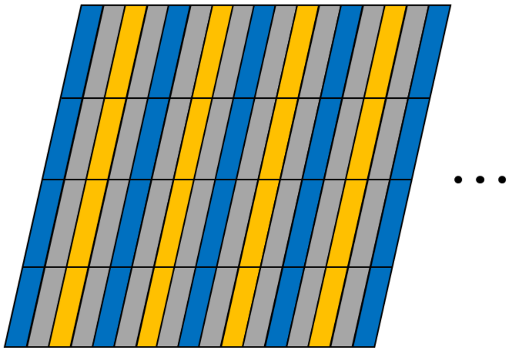


Figure 12: Plates Specification of LEU Fuel Elements

- F plates:
  - Height: 3.5520 cm
  - Thickness: 0.0635 cm
  - Width: 1.3221 cm
  - Volume: 0.2982 cm^3
- Y plates:
  - Height: 3.5520 cm
  - Thickness: 0.0432 cm
  - Width: 1.3221 cm
  - Volume: 0.2028 cm^3
- T plates:
  - Height: 3.5520 cm
  - Thickness: 0.0330 cm
  - Width: 1.3221 cm
  - Volume: 0.1551 cm^3

Moreover, MCODE-FM creates one new universe per defined fuel element in the *mcode_input* file, starting with universe 1, and then fills each core position (cells 101 to 127) with the corresponding universe. MCODE-FM also writes fuel elements cell importances (imp:n=1) and temperatures (tmp=3.2154e-8) in a vertical format, as well as tally materials and flux tallies.

The *mc000i* file created by MCODE-FM as the initial fresh LEU core model is also used as the MCNP input for ADDER calculations, after undergoing a few modifications as described in 3.1.1.2.

3.1.3. In-Core Experiments (ICE)

3.1.3.1. ICE Simplified Geometry

As described in 1.2.1, simplified In-Core Experiments (ICE) can be inserted in positions A1, A3 and B3 of the MITR core. In order to more accurately model typical MITR operations, a simplified ICE geometry is selected to assess the impact of such a change in the core geometry, especially given its small size.

The simplified ICE geometry is based on the aluminum dummy element with inset per R3F-15-4B (universe 35), which is the dummy inserted in positions A1, A3, B3, B6 and B9 of the fresh HEU and LEU cores when no ICE is inserted. This dummy element presents a cylindrical hole (radius of 0.397 cm) to allow for water bypass. A larger hole radius (1.03 inches / 2.618 cm) is selected for the ICE geometry to accommodate an experimental sample. The sample is a homogeneous cylinder filled with a material relevant to MITR in-core irradiation. The dummy hole is filled with helium above and below the sample (see Figure 13), which is assumed to be at 323.15K (2.7847E-8 MeV, tmp card in the MCNP model) and atmospheric pressure, and therefore to have a density of 0.000149 g/cm^3.

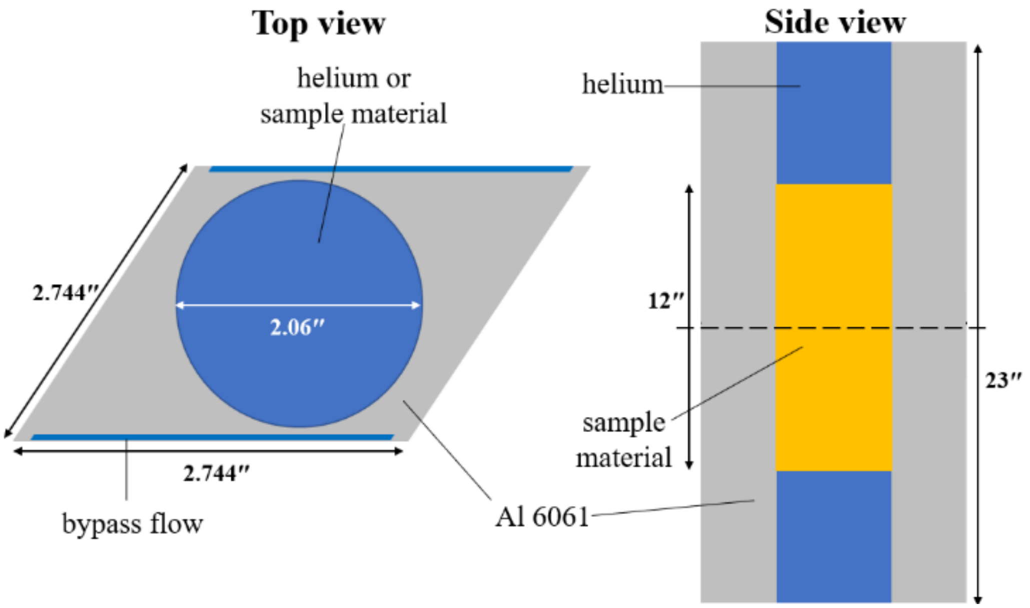


Figure 13: Simplified ICE Geometry

The sample is made of a material that has been irradiated in the MITR. The selected materials of interest for this study are pressurized light water, graphite, tungsten and FLiBe, whose properties are summarized in Table 4.

Table 4: ICE Sample Materials Properties

In-Core Experiment	Isotopes	Molecules	Temperature (°C / MeV)	Pressure (MPa)	Density (g/cm^3)	Comments
Pressurized Water Loop (W)	H ; O	H_2O	300 / 4.939E-8	10	0.7 [23]	PWR pressure
Graphite (G)	C	C	700 / 8.3847E-8	X	1.8 [24]	Solid: assume constant density Nuclear grade graphite
Tungsten (T)	W	W	800 / 9.2477E-8	X	19.3 [25]	Solid: assume constant density
FLiBe (F)	F ; Li ; Be	LiF ; BeF_2	700 / 8.3847E-8	0.1	1.9 [26]	67% LiF – 33% BeF_2 [26] 99.99% of Li-7 [27]

The height of the sample was selected based on the analysis described in 4.1.2, in order for the ICE to bring a significant reactivity effect while allowing for the shim bank to stay within the operational range (withdrawal between 12.70 and 53.34 cm, cf. 2.3.2). The pressurized water, graphite and FliBe samples are 12 inches long, and the tungsten sample is 1.5 inches long.

3.1.3.2. ICE Modelling

As described previously, the simplified ICE geometry is based on the dummy element with inset per R3F-15-4B geometry, which is described in universe 35 in the *skeleton_input* file.

This model is modified by increasing the cylindrical hole radius to 1.03 inches (2.618 cm) to accommodate the experimental sample. Moreover, the inside of the cylinder is divided into three parts: top helium, sample material and bottom helium. The ICE is described in universe 40, which is added to the *skeleton_input* file. The ICE is then inserted in different positions of the core (A-1, A-3 or B-3) by specifying “40” after the **universe** card (cf. 3.1.1.2).

3.2.Core Cycle Length Description

As described in 2.3.1.2, MCODE-FM’s default behavior for MITR calculations consists in the following depletion steps, hardcoded into the MCODE script *subs.py* to capture the Xenon peak at the beginning of the cycle:

If the cycle is less than 40 days: day 0, day 1, day 3, end of cycle
If the cycle is more than 40 days: day 0, day 1, day 3, day 40, end of cycle

Similar depletion steps are selected for ADDER calculations to carry out the code-to-code comparison. Selected depletion options (ORIGEN version, ORIGEN cross section and decay libraries, predictor-corrector methods, nuclide selection process), are described in 2.3 for both ADDER and MCODE.

The selected MCODE depletion options are either default options – predictor-corrector method, number of depletion substeps (20), ORIGEN cross sections update – or hardcoded into the MCODE-FM script *subs.py* – PWRUE.LIB, neutron absorption fraction threshold (0.999).

The selected ADDER depletion options are described at the beginning of the *adder_input* file, and are used for all timesteps (cf. Appendix A).

3.2.1. 7 Days at Full Power

7-day calculations at full power were first carried out to make sure that both softwares were running correctly.

The MCODE-FM cycle description (power and timesteps) is specified at the beginning of the *mcode_input* file. The power is entered in watts, and the time in days. The only difference between the fresh HEU and the fresh LEU cores are the power levels, respectively 5.7 MW and 7 MW.

The fresh HEU core and fresh LEU core MCODE-FM 7-day cycle descriptions are presented in Appendix A.

The successive ADDER operations (depletion and critical search) are described in the *adder_input* file. Each depletion step requires a duration (in days) and a power level (in MW). Each critical search requires a target k_{eff} (1 to achieve criticality), a shim bank height range (12.70-53.34 cm) and a tolerance (cf. 2.3.2).

The fresh HEU core and fresh LEU core ADDER 7-day cycle descriptions are presented in Appendix A.

3.2.2. Full 10-week Cycle at Full Power

A more representative MITR cycle consists in 10 weeks / 70 days at full power, as explained in 1.2.3.1. This type of cycle was selected as the main cycle type for code-to-code comparison between MCODE and ADDER.

The fresh HEU core and fresh LEU core MCODE-FM and ADDER 70-day cycle descriptions are presented in Appendix A.

3.2.3. Full Cycle at Full Power with Mid-Cycle Restart

During a full operating cycle, the MITR might be shut down for a limited period of time, either due to unpredictable conditions or to insert / remove an in-core experiment, before restarting. An additional type of cycle, which includes such a mid-cycle restart, is therefore studied in this work. The selected cycle consists in 7 days at full power to attain xenon equilibrium, followed by 7 hours at 100 kW to capture the Xenon peak (see Figure 14), and another 7 hours at full power to model the restart [28]. The study will focus on tracking Xenon evolution and shim bank height throughout the mid-cycle restart.

The MCODE-FM script *subs.py* was modified to divide the 7-hour low power step into 14 30-minute steps to accurately track the evolution of Xenon worth and capture its peak.

The timesteps in the *mcode_input* file are specified cumulatively in days, and both 7-day periods are subdivided into the 0 / 1 / 3 / 7 days MCODE-FM default depletion scheme (cf. 2.3.1.2). The 7-hour period corresponds to 0.29167 day.

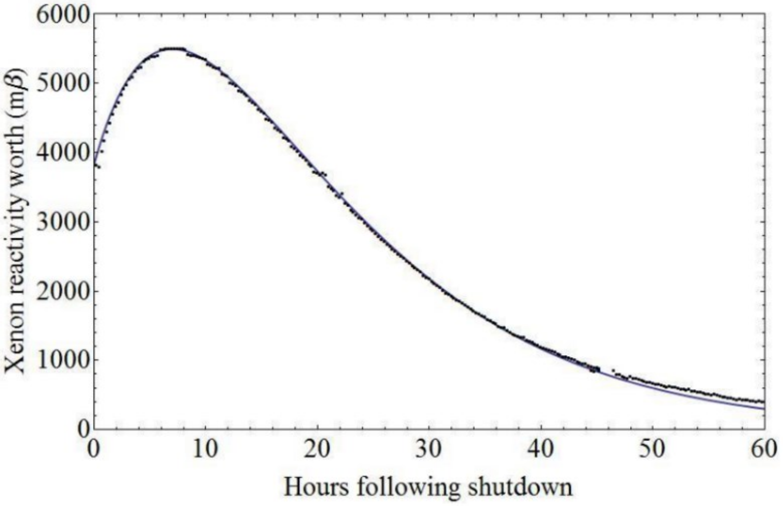


Figure 14: MITR Shutdown Xenon Worth Transient After Equilibrium Operation at 5.7 MW [28]

The fresh HEU core and fresh LEU core MCODE-FM 70-day cycle with mid-cycle restart descriptions are presented in Appendix A.

The ADDER input is modified to follow the MCODE-FM depletion scheme described in 3.2.3.1. The fresh HEU core and fresh LEU core ADDER 70-day cycle with mid-cycle restart descriptions are presented in Appendix A.

3.3. Selected Core Parameters and Nuclides for Comparison

3.3.1. Global Quantities

The main global quantities to compare between MCODE and ADDER results are the k_{eff} and the shim bank height.

The MCODE- and ADDER-computed k_{eff} will always be close to one another, because the target k_{eff} is 1 in all calculations and the selected tolerances are identical (100 pcm, cf. 2.3).

The shim bank height is specified in output files in centimeters. It can range from the subcritical interlock position (12.70 cm / 5 inches) to the full-out position (53.34 cm / 21 inches), with a typical end-of-cycle position of 45.72 cm / 18 inches for a 70-day cycle at full power (cf. 1.2.3.1). More relevant shim bank height comparisons can be carried out by using the shim bank worth curves, to assess the height difference as a worth difference, which can then be compared to the k_{eff} difference or the selected k_{eff} tolerance. The shim bank worth calculations are described in 4.3.

3.3.2. Local Quantities

The following local quantities will be compared between MCODE and ADDER results to assess good agreement between the two softwares:

- Neutron flux
- Atom inventory:
    - Actinides: U-235, U-236, Pu-239, Np-237
    - Neutron poisons: Xe-135, Sm-149
- Power density distribution
- Fission density distributions

The neutron flux is particularly relevant to compare because of its importance for in-core irradiation.

The three selected actinides are tracked as part of the MITR fuel management, which requires monitoring the inventory of Special Nuclear Materials (SNM). An uncertainty of up to 5g of U-235 per fuel element at end of life in core is considered as acceptable during fuel management calculations. Assuming that fuel elements usually spend 10 cycles into the core, an uncertainty below 0.5 g of U-235 can be considered as acceptable after one cycle for HEU cases (linear extrapolation). Neutron poisons have an impact on the MITR operation – especially during shutdown (and eventual restart) – and their inventory will therefore be analyzed.

Moreover, the power density distribution is typically relevant as input data for thermal hydraulics calculations.

Finally, the fission density is one of the MITR neutronics safety limits, which are described in 1.2.3.2 (HEU) and 1.3.2 (LEU). An uncertainty below ~10% of the safety limit on cumulative fission densities (from an element's insertion in the core to its removal) is considered as acceptable during fuel management calculations. Assuming that fuel elements usually spend 10 cycles into the core, an uncertainty below ~1% of the safety limit can be considered as acceptable after one cycle for HEU cases (linear extrapolation).

4. MCODE and ADDER Results Comparison

Before modelling full cycles, preliminary calculations need to be carried out to efficiently analyze results (shim bank worth) and make relevant choices for the MITR model (in-core experiments position and sample length, number of simulated neutrons and cycles).

4.1. Shim Bank Worth

Converting shim bank height differences from centimeters to pcm will facilitate the assessment of good agreement between MCODE and ADDER. Indeed, a worth difference can be compared to other quantities, such as the critical search tolerance (cf. 2.3.1.2), or the overall reactivity of the core (gap to criticality). In order to do so, the integral shim bank worth must be computed with MCNP.

4.1.1. MCNP Methodology

To compute the MITR integral shim bank worth, successive MCNP5 kcode calculations are carried out where the shim bank is initially fully inserted, and gradually raised until it reaches its full-out position. Each withdrawal increment is equal to 2.54 cm, which requires 22 MCNP calculations. The shim bank worth is then determined by the difference in k_{eff} ($k_{eff,z} - k_{eff,z=0}$) between the current height and the fully inserted case.

The shim bank worth is computed for two configurations: fresh HEU core without any ICE, and fresh LEU core without any in-core experiment (ICE). The MCNP models are described in 3.1.1.2 and 3.1.2.2. The results will then be used respectively for all HEU and LEU shim bank heights analyses.

4.1.2. Fresh HEU Core Shim Bank Worth

The MCNP5 calculations yield the following shim bank worth for the fresh HEU core:

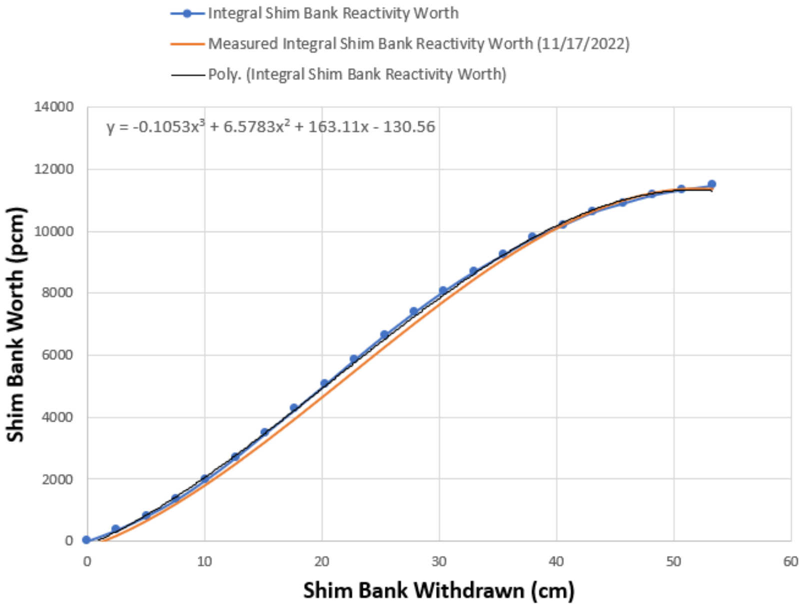


Figure 15: Integral Shim Bank Worth – Fresh HEU Core (σ~10 pcm)

For comparison, the latest available measured shim bank worth (Nov 17, 2022) can be modelled by the following polynomial (shown in orange in Figure 15) [29]:

$$y = -0.1142x^3 + 7.6291x^2 + 135.03x - 213.52$$

4.1.3. Fresh LEU Core Shim Bank Worth

The MCNP5 calculations yield the following shim bank worth for the fresh LEU core:

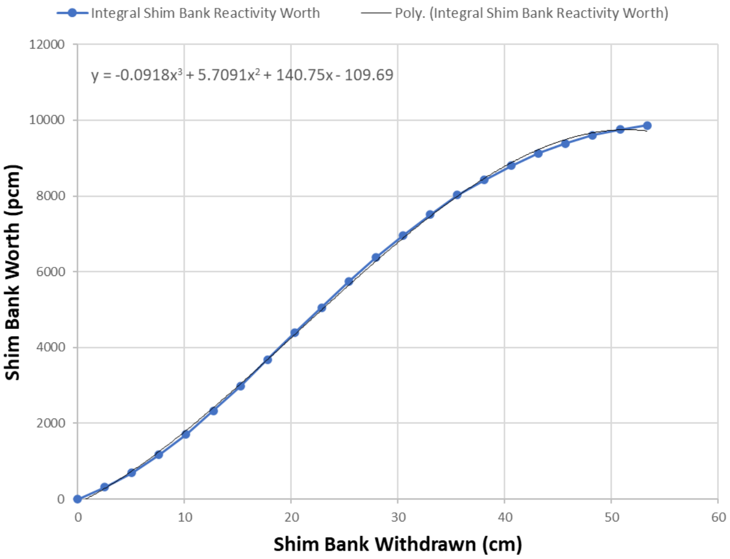


Figure 16: Integral Shim Bank Worth – Fresh LEU Core (σ~10 pcm)

4.2.Modelling Parameters Analyses

Preliminary studies were carried out to select relevant ICE positions, ICE samples lengths and MCNP kcode card by comparing shim bank heights using the previously computed shim bank worths.

4.2.1. ICE Sample Length

The simplified ICE geometry is described in 3.1.3.1. The sample length must be selected to introduce a non-negligible perturbation in the core, to justify studying different cases. However, this perturbation must allow for the shim bank to maintain the core critical while remaining in its operational height range (0-53.34 cm). For instance, an ICE that represents a large negative reactivity insertion could keep the core subcritical, even after full withdrawal of the shim bank.

Sample lengths of 4, 8, 12 inches were initially analyzed for pressurized water and graphite. The samples were inserted in position A-1 of a fresh HEU core. 7-day calculations at full power were carried out using MCODE, and the final shim bank height was compared to a reference case (fresh HEU core without any in-core experiment). The difference was converted from centimeters to pcm using the shim bank worth presented in 4.1.2. The results are presented in Table 5, and the selected lengths are shown in bold.

Table 5: ICE Sample Length Selection (σ~30 pcm)

In-Core Experiment	Sample Length	EOC Shim Bank Height (cm)	Shim Bank Worth Difference at day 7 (pcm)
No ICE	N/A	33.754	N/A
Pressurized Water	4 inches	33.794	-10
	8 inches	33.730	6
	12 inches	**33.057**	**174**
Graphite	4 inches	34.467	-174
	8 inches	33.633	30
	12 inches	**33.265**	**122**
FLiBe	4 inches	33.979	-55
	8 inches	33.833	-20
	12 inches	**33.405**	**87**
Tungsten	2 inches	37.025	-761
	4 inches	38.964	-1163
	6 inches	41.957	-1695
	12 inches	50.527	-2502

A 12-inch length was selected for the pressurized water, graphite and FLiBe samples. However, the shim bank worth differences caused by the tungsten sample are large enough to potentially keep the core subcritical at EOC for a 70-day cycle.

Additional MCODE calculations were therefore carried out to determine an acceptable tungsten sample length, where a 70-day cycle at full power is simulated. The sample length was decreased until the final shim bank height was sufficiently lower than the full-out position (53.34 cm). The results are presented in Table 6, and the selected length is shown in bold.

Table 6: Tungsten ICE Sample Length Selection (σ~30 pcm)

In-Core Experiment	Sample Length	EOC Shim Bank Height (cm)
Tungsten	2 inches	53.208
	1.75 inches	53.070
	1.5 inches	**51.164**

A 1.5-inch length is selected for the tungsten sample.

4.2.2. ICE Positions

As described in 1.2.1, ICEs can be inserted in positions A-1, A-3 and B-3. To reduce the number of calculations required for the feasibility assessment, it is assumed that ICEs will have a similar impact on the core whether they are inserted in positions A-1 or A-3 (A-ring).

To justify this assumption, 7-day calculations at full power are carried out using MCODE for fresh HEU core configurations, where ICEs are inserted into positions A-1 and A-3. The ICE sample lengths selected in 4.2.1 are used for these calculations. The shim bank height differences were converted from centimeters to pcm using the shim bank worth presented in 4.1.2. The results are presented in Table 7.

Table 7: Comparison between A-1 and A-3 ICE Positions (σ~30 pcm)

In-Core Experiment	Day	A-1 Shim Bank Height (cm)	A-3 Shim Bank Height (cm)	Shim Bank Worth Difference (pcm)
Pressurized Water 12 inches	0	21.783	21.662	-36
	1	29.863	29.969	29
	3	32.251	31.916	-87
	7	33.057	33.045	-3
Graphite 12 inches	0	22.014	21.831	-55
	1	30.607	30.096	-139
	3	32.230	32.355	32
	7	33.265	33.666	100
FLiBe 12 inches	0	21.923	21.884	-12
	1	30.290	30.629	92
	3	32.171	32.346	45
	7	33.405	33.250	-39
Tungsten 1.5 inches	0	24.365	24.318	-14
	1	32.786	32.855	18
	3	35.572	35.671	23
	7	36.582	36.494	-20

The shim bank worth difference stays below 200 pcm in all cases, which corresponds to the selected tolerance interval for the critical shim bank height search algorithm (cf. 2.3.1.2). Moreover, for all cases, the shim bank worth difference does not increase throughout the 7-day cycle. The difference between positions A-1 and A-3 impact on core reactivity can therefore be considered as negligible.

In the following calculations, ICEs will be inserted in positions A-1 and B-3 to test their impacts in both rings, but not in position A-3 to reduce the number of simulations to carry out.

4.2.3. kcode Card

The typical kcode card used in MCODE calculations is the following (written in the *skeleton_input* file):

```
kcode   100000 1.12 30 200
```

This kcode card yields k_{eff} results with standard deviations usually ranging from 20 to 35 pcm for the MITR model, which is satisfactory for routine fuel management calculations.

However, this kcode card induces a larger error on reaction rates, which need to be precisely computed to accurately carry out depletion calculations. A compromise therefore needs to be found between increasing the number of simulated neutrons and the duration of the simulation.

Due to the lateral segmentation of fuel plates, which is selected for LEU core configurations but not for HEU core configurations (cf. Chapter 3), fuel cells are smaller in LEU models. Consequently, the number of neutrons interacting in each cell is lower for LEU cases, which increases the error on reaction rates. The kcode card analysis is therefore carried out using the fresh LEU core model (without any ICE) described in 3.1.2.2. The calculations are carried out using ADDER to model a 70-day cycle at full power (7 MW_{th}).

The following kcode cards are selected for this analysis:

1. 1,000,000 neutrons per cycle; 200 cycles; 30 inactive cycles
2. 500,000 neutrons per cycle; 200 cycles; 30 inactive cycles
3. 100,000 neutrons per cycle; 200 cycles; 30 inactive cycles
4. 1,000,000 neutrons per cycle; 100 cycles; 20 inactive cycles
5. 500,000 neutrons per cycle; 100 cycles; 20 inactive cycles
6. 100,000 neutrons per cycle; 100 cycles; 20 inactive cycles

The other parameters of the kcode card are kept as the default values described in [13] (except for the number of source points for which to allocate storage, which was set to 20,000):

- Initial guess for keff: 1.00000
- Normalization of tallies: by weight (0)
- Maximum number of cycle values on MCTAL or RUNTPE files: 6,500
- Number of cycles over which summary and tally information are averaged: average over active cycles only (1)

For each case, the EOC MCNP file is analyzed to extract the average and maximum relative error for key reaction rates. The following nuclide-reaction combinations are selected:

- U-235 / (n,γ)
- U-235 / fission
- U-238 / (n,γ)
- U-238 / fission
- Pu-239 / (n,γ)
- Pu-239 / fission
- Xe-135 / (n,γ)
- Sm-149 / (n,γ)

The results are presented in Table 8. The nuclide-reaction combination that shows the highest relative error (average and maximum) on reaction rates for all cases is U-238 / (n,γ). For this study, maximum relative error is considered as acceptable up to ~10% for key reaction rates, which is respected by cases 1, 2 and 4. The elapsed time for case 1 is significantly higher than for cases 2 and 4. Case 2 can therefore be selected, as it achieves the same accuracy as case 4 in a shorter amount of time.

The selected kcode for all calculations described below is:

```
kcode   500000 1.00000 30 200 20000 0 6500 1
```

Table 8: Reaction Rates Errors for the kcode Card Analysis

Case	Elapsed Time	Nuclide	Reaction	Average Relative Error	Maximum Relative Error
1	58:52:40	U-235	(n,γ)	0.48%	0.85%
			fission	0.50%	0.87%
		U-238	**(n,γ)**	**3.41%**	**6.59%**
			fission	0.43%	0.86%
		Pu-239	(n,γ)	0.68%	1.12%
			fission	0.60%	0.99%
		Xe-135	(n,γ)	0.64%	1.12%
		Sm-149	(n,γ)	0.66%	1.18%
2	**30:54:47**	U-235	(n,γ)	0.69%	1.23%
			fission	0.71%	1.23%
		U-238	**(n,γ)**	**4.82%**	**10.44%**
			fission	0.61%	1.18%
		Pu-239	(n,γ)	0.96%	1.56%
			fission	0.84%	1.36%
		Xe-135	(n,γ)	0.90%	1.57%
		Sm-149	(n,γ)	0.94%	1.66%
3	10:32:38	U-235	(n,γ)	1.53%	3.15%
			fission	1.58%	2.88%
		U-238	**(n,γ)**	**10.49%**	**33.61%**
			fission	1.37%	2.65%
		Pu-239	(n,γ)	2.14%	3.75%
			fission	1.88%	3.30%
		Xe-135	(n,γ)	2.02%	3.60%
		Sm-149	(n,γ)	2.10%	3.87%
4	41:42:43	U-235	(n,γ)	0.71%	1.28%
			fission	0.73%	1.28%
		U-238	**(n,γ)**	**4.95%**	**10.60%**
			fission	0.63%	1.23%
		Pu-239	(n,γ)	0.99%	1.56%
			fission	0.87%	1.40%
		Xe-135	(n,γ)	0.93%	1.65%
		Sm-149	(n,γ)	0.97%	1.74%
5	22:36:19	U-235	(n,γ)	1.00%	1.77%
			fission	1.03%	1.77%
		U-238	**(n,γ)**	**6.97%**	**17.06%**
			fission	0.90%	1.75%
		Pu-239	(n,γ)	1.40%	2.37%
			fission	1.23%	2.05%
		Xe-135	(n,γ)	1.32%	2.46%
		Sm-149	(n,γ)	1.37%	2.57%
6	9:36:14	U-235	(n,γ)	2.23%	4.47%
			fission	2.30%	4.12%
		U-238	**(n,γ)**	**15.02%**	**41.60%**
			fission	2.00%	4.10%
		Pu-239	(n,γ)	3.10%	5.82%
			fission	2.74%	4.98%
		Xe-135	(n,γ)	2.94%	5.48%
		Sm-149	(n,γ)	3.06%	6.13%

4.3. Post-Processing Scripts

Python scripts were developed to extract data from MCODE and ADDER output files, and to visualize differences between the outputs.

4.3.1. Data Extraction Scripts

4.3.1.1. MCODE Data Extraction

MCODE produces several output files, including a text file *output_file*, which describes the different shim bank heights that were tested during the critical searches, as well as the corresponding k_{eff} and standard deviations. Moreover, MCODE saves the isotopic composition of each material to a separate .PCH file (text format). For each depletion step, three .PCH files are created: a predictor file, a corrector file, and an average of both steps (cf. 2.3.1.1). The flux used to deplete the material is also specified at the end of the .PCH file.

Two scripts are written to extract data from MCODE results and build adequate Python dictionaries that can be used by visualizations scripts (cf. 4.3.2). *get_MCODE_global_results.py* allows reading of the shim bank height, k_{eff} and standard deviation for each step in the *output_file* file, while *get_MCODE_local_results_HEU.py* and *get_MCODE_local_results_LEU.py* read fluxes and nuclide inventories from the appropriate .PCH files.

4.3.1.2. ADDER Data Extraction

ADDER produces two output files: *adder.log* and *adder_results.h5*.

The *adder.log* file (text format) keeps a record of all messages from ADDER, as well as the date and time when each operation was carried out. It is updated throughout the calculation and used to monitor its progress.

The *adder_results.h5* (HDF5 format) contains all results for each step of the calculation, and its structure is described in [9].

However, the current version of ADDER (v1.0.1) presents a bug that prevents the correct storage of the k_{eff} standard deviation for critical search steps. The k_{eff} and its standard deviation are therefore extracted from the *adder.log* file.

A first script, *get_ADDER_global_results.py*, was written to extract the global results of a case, i.e. k_{eff}, its standard deviation and shim bank height for all steps of the calculation. All results are extracted from the *adder.log* file to make sure that the correct k_{eff} standard deviation is stored in the results Python dictionary. Two other scripts, *get_ADDER_local_results_HEU.py* and *get_ADDER_local_results_LEU.py*, allow to extract local results respectively for MITR HEU and LEU models. All resulting Python dictionaries can be used by visualization scripts (cf. 4.3.2.1).

4.3.2. Visualization Scripts

Python scripts were written to facilitate the visualization of ADDER-MCODE differences.

Global results, such as shim bank heights, k_{eff} and Xe-135 and Sm-149 atom inventories over the whole core, are plotted on separate graphs.

Local results, such as flux and fission densities, are plotted on two different types of figures to visualize the spatial distribution of the differences between the two software results.

Flux and fission densities are plotted on a MITR core map which shows each plate (and each lateral node for the LEU core). For each plate, the results are first averaged over all axial nodes for both MCODE and ADDER, before computing the relative difference using the following formula:

$$relative\ difference = \frac{ADDER\ averaged\ result - MCODE\ averaged\ result}{MCODE\ averaged\ result} \times 100\%$$

These two types of results are also plotted for each fuel element, to visualize the axial dependency of the relative difference. For each axial node, the results are first averaged over all plates for both MCODE and ADDER, before computing the relative difference using the same formula as described above.

U235 atom inventory is treated differently, to easily check if the difference in results stays below the acceptable uncertainty on U235 mass per element. A simplified MITR core map is plotted where the difference in U235 mass is specified in grams for each fuel element.

Finally, the node presenting the largest relative difference between ADDER and MCODE results will be presented to give a sense of the order of magnitude of local differences, which cannot be perfectly captured by the core map and fuel element visualization.

4.4.7 Days at Full Power

As a first step, a 7-day cycle at full power is modelled in ADDER and MCODE to troubleshoot problems encounter when first running both software, and assess the agreement of shim bank heights over a short cycle.

The fresh HEU core configuration used for this analysis is described in 3.1.1, except for the kcode card which presents the same options that are used for MITR fuel management calculations (`100000 1.12 30 200`). Its MCNP model is built by MCODE-FM at the beginning of the MCODE calculation, and reused as an input file for the ADDER calculation. The four types of ICEs described in 3.1.3 are successively inserted in positions A-1 and B-3 according to the conclusion of the analysis described in 4.2.2.

The calculations are identified by a two or three-character ID, as described in Table 9. The ID can be followed by "_7", "_70" and "_restart" to respectively describe the 7-day cycle at full power, the 70-day cycle at full power and the mid-cycle restart calculations (see 3.2).

Table 9: Calculations ID

Case ID	MITR Core	ICE Type	ICE Position
H0	Fresh HEU Core	None	N/A
HFA		FLiBe	A-1
HFB			B-3
HGA		Graphite	A-1
HGB			B-3
HTA		Tungsten	A-1
HTB			B-3
HWA		Pressurized Water	A-1
HWB			B-3

L0	Fresh LEU Core	None	N/A
LFA		FLiBe	A-1
LFB			B-3
LGA		Graphite	A-1
LGB			B-3
LTA		Tungsten	A-1
LTB			B-3
LWA		Pressurized Water	A-1
LWB			B-3

Shim bank heights and k_{eff} results of the 7-day cycle ADDER and MCODE calculations are presented in Table 10. Shim bank height differences are converted to worth differences by using the HEU shim bank worth presented in 4.1.2.

MCODE and ADDER k_{eff} results are always within 200 pcm of each other thanks to the ± 100 pcm tolerance set for critical searches (cf. Chapter 2).

MCODE and ADDER shim bank height results are also within 200 pcm of each other, and do not increase after each depletion step, which shows good agreement between the two software for this metric, for all types and positions of ICE. The highest worth difference (-132 pcm) is attained for case HGB at day 7.

This preliminary analysis allows confirmation of the ADDER options selected to model calculations in a similar way as the MCODE options used for the MITR fuel management. These ADDER options will be kept for 70-day cycle and mid-cycle restart calculations.

This preliminary analysis was only carried out with the fresh HEU core, because the fresh LEU core 70-day cycle and mid-cycle restart calculations will use the same MCODE and ADDER options. Moreover, 70-day cycle calculations will help assess the fact that the fresh LEU core was correctly built by MCODE-FM script *subs.py* after it was modified to support the MITR LEU fuel element design. To that end, the EOC shim bank height will be compared to the predicted EOC shim bank height for equilibrium all-LEU cores in [7].

Table 10: k_{eff} and Shim Bank Height Comparison for Fresh HEU Core / 7-day Cycle

Case ID	Day	MCODE k_{eff}	ADDER k_{eff}	k_{eff} Difference (pcm)	MCODE Shim Bank Height (cm)	ADDER Shim Bank Height (cm)	Worth Difference (pcm)
H0_7	0	1.00020 +/- 0.00028	0.99979 +/- 0.00029	-41	22.361	22.393	10
	1	0.99969 +/- 0.00028	0.99975 +/- 0.00030	6	30.544	30.715	46
	3	0.99983 +/- 0.00029	1.00023 +/- 0.00030	40	32.764	32.994	58
	7	0.99969 +/- 0.00028	1.00005 +/- 0.00027	36	33.754	33.651	-26
HFA_7	0	0.99998 +/- 0.00031	1.00037 +/- 0.00028	39	21.923	22.031	32
	1	1.00030 +/- 0.00034	1.00026 +/- 0.00026	-4	30.290	30.274	-4
	3	0.99966 +/- 0.00029	0.99988 +/- 0.00031	22	32.171	32.481	80
	7	0.99986 +/- 0.00029	1.00015 +/- 0.00029	29	33.405	33.399	-2
HFB_7	0	0.99947 +/- 0.00028	1.00015 +/- 0.00031	68	21.895	22.000	31
	1	1.00061 +/- 0.00028	0.99983 +/- 0.00028	-78	30.586	30.322	-71
	3	0.99972 +/- 0.00025	1.00036 +/- 0.00029	64	32.417	32.439	6
	7	0.99948 +/- 0.00029	1.00030 +/- 0.00021	82	33.376	33.480	26
HGA_7	0	0.99937 +/- 0.00029	1.00039 +/- 0.00027	102	22.014	22.004	-3
	1	1.00065 +/- 0.00028	1.00000 +/- 0.00022	-65	30.607	30.266	-92
	3	0.99943 +/- 0.00027	1.00007 +/- 0.00029	64	32.230	32.400	44
	7	0.99977 +/- 0.00026	1.00029 +/- 0.00028	52	33.265	33.023	-61
HGB_7	0	1.00002 +/- 0.00028	1.00007 +/- 0.00028	5	21.961	22.006	13
	1	1.00010 +/- 0.00032	0.99978 +/- 0.00028	-32	30.462	30.170	-79
	3	0.99954 +/- 0.00027	0.99977 +/- 0.00034	23	32.293	32.271	-6
	7	**1.00068 +/- 0.00023**	**0.99970 +/- 0.00025**	**-98**	**33.933**	**33.401**	**-132**
HTA_7	0	1.00058 +/- 0.00031	0.99995 +/- 0.00031	-63	24.365	24.271	-28
	1	0.99935 +/- 0.00031	1.00051 +/- 0.00023	116	32.786	33.109	82
	3	1.00047 +/- 0.00026	0.99992 +/- 0.00029	-55	35.572	35.405	-39
	7	1.00002 +/- 0.00028	1.00029 +/- 0.00022	27	36.582	36.490	-20
HTB_7	0	1.00004 +/- 0.00034	0.99996 +/- 0.00035	-8	24.286	24.468	54
	1	0.99948 +/- 0.00032	0.99995 +/- 0.00026	47	33.011	33.042	8
	3	0.99959 +/- 0.00028	1.00021 +/- 0.00030	62	35.154	35.690	125
	7	0.99949 +/- 0.00031	1.00027 +/- 0.00028	78	36.435	36.575	31
HWA_7	0	1.00069 +/- 0.00028	1.00012 +/- 0.00031	-57	21.783	21.506	-83
	1	0.99980 +/- 0.00033	0.99959 +/- 0.00029	-21	29.863	29.830	-9
	3	0.99983 +/- 0.00027	0.99956 +/- 0.00027	-27	32.251	31.997	-66
	7	1.00030 +/- 0.00031	1.00032 +/- 0.00027	2	33.057	32.918	-35
HWB_7	0	1.00008 +/- 0.00031	1.00014 +/- 0.00029	6	20.671	20.633	-11
	1	1.00035 +/- 0.00030	1.00048 +/- 0.00025	13	29.263	29.157	-29
	3	0.99983 +/- 0.00030	1.00018 +/- 0.00030	35	30.990	31.031	11
	7	0.99969 +/- 0.00028	0.99992 +/- 0.00031	23	32.134	32.054	-21

4.5. Full Cycle at Full Power

As described in 3.2.2, a 70-day cycle at full power is selected to model a typical MITR cycle for both HEU and LEU cores. The calculations IDs are described in Table 9.

4.5.1. Fresh HEU Core Results

4.5.1.1. Global Results

The fresh HEU core configuration used for this analysis is described in 3.1.1.

Shim bank heights and k_{eff} results of the 70-day cycle ADDER and MCODE calculations are presented in Table 11. Shim bank height differences are converted to worth differences by using the HEU shim bank worth presented in 4.1.2. For reference, shim blades height are experimentally measured in inches, with two significant digits after the decimal point.

MCODE and ADDER k_{eff} results are always within 200 pcm of each other thanks to the ± 100 pcm tolerance set for critical searches (cf. Chapter 2). For ADDER calculations, the number of simulated neutrons is adapted during the critical search to optimize the calculation duration, leading to higher standard deviations (compared with MCODE). After the search, a new MCNP calculation is carried out by ADDER with the adequate shim bank height to compute fluxes and reaction rates used for depletion (predictor step), with the user-specified kcode card. Such MCNP calculations have lower standard deviations, closer to MCODE ones (~10 pcm). Their k_{eff} and standard deviations are presented in Table 11, except for the end of cycle, for which the last results of the critical search are presented because this search is not followed by a depletion calculation.

MCODE and ADDER shim bank height results are also within 200 pcm of each other, and do not increase after each depletion step, which shows good agreement between the two software for this metric, for all types and positions of ICE. The highest worth difference (78 pcm) is reached by case HFA at day 40.

4.5.1.2. Local Results

As described in 3.3.2, the relevant local results to analyze are the one-group integral neutron flux, the cumulative fission densities and the inventories of relevant actinides and neutron poisons. In the data extraction scripts described in 4.3.1, fission densities and power densities are both deduced from the difference in total actinide inventories before and after a depletion step, and would therefore present the same relative differences. This study therefore focuses on fission densities to compare MCODE and ADDER results, considering that results can be compared to the acceptable uncertainty on end-of-life cumulative fission densities described in 3.3.2.

The maximum difference and its location (element / plate / axial node) are presented in Table 12 for the different result types for fresh HEU cases at EOC, except for actinides inventories, where relative differences will be described per fuel element. The EOC neutron flux analyzed here is the one-group flux used for the last depletion step (before the final critical shim bank height search).

For neutron flux and Xe-135 and Sm-149 atom inventories, the relative difference is presented by using the following formula:

$$relative\ difference = \frac{ADDER\ result - MCODE\ result}{MCODE\ result} \times 100\%$$

For cumulative fission densities, the difference between ADDER and MCODE results is presented in fis/cm^3 (between BOC and EOC) to facilitate the comparison with the acceptable uncertainty criterion described in 3.3.2, which is equal to ~1.8 x 10^{19} fis/cm^3 for one full cycle for the HEU core.

Table 11: k_{eff} and Shim Bank Height Comparison for Fresh HEU Core / 70-day Cycle

Case ID	Day	MCODE k_{eff}	ADDER k_{eff}	k_{eff} Difference (pcm)	MCODE Shim Bank Height (cm)	ADDER Shim Bank Height (cm)	Worth Difference (pcm)
H0_70	0	1.00007 +/- 0.00012	1.00042 +/- 0.00010	35	22.359	22.398	12
	1	1.00081 +/- 0.00011	1.00036 +/- 0.00010	-45	31.040	30.851	-51
	3	1.00048 +/- 0.00015	1.00008 +/- 0.00009	-40	33.206	32.926	-71
	40	0.99927 +/- 0.00011	1.00025 +/- 0.00010	98	40.238	40.562	58
	70	1.00023 +/- 0.00013	1.00015 +/- 0.00024	-8	46.056	45.395	-69
HFA_70	0	0.99984 +/- 0.00013	1.00022 +/- 0.00010	38	21.955	21.981	8
	1	0.99982 +/- 0.00014	1.00026 +/- 0.00010	44	30.181	30.270	24
	3	0.99967 +/- 0.00014	1.00031 +/- 0.00009	64	32.383	32.475	24
	40	**0.99922 +/- 0.00012**	**1.00043 +/- 0.00009**	**121**	**39.556**	**39.972**	**78**
	70	0.99928 +/- 0.00014	1.00050 +/- 0.00021	122	44.367	44.618	31
HFB_70	0	0.99994 +/- 0.00014	1.00047 +/- 0.00010	53	21.905	22.072	50
	1	0.99987 +/- 0.00013	1.00015 +/- 0.00010	28	30.245	30.236	-2
	3	0.99943 +/- 0.00011	1.00020 +/- 0.00010	77	32.324	32.459	35
	40	0.99918 +/- 0.00009	0.99990 +/- 0.00009	72	39.554	39.540	-3
	70	0.99943 +/- 0.00014	0.99979 +/- 0.00029	36	44.483	44.494	1
HGA_70	0	0.99992 +/- 0.00016	1.00010 +/- 0.00010	18	21.982	21.977	-1
	1	1.00073 +/- 0.00013	1.00064 +/- 0.00009	-9	30.632	30.421	-57
	3	0.99977 +/- 0.00013	1.00005 +/- 0.00010	28	32.423	32.398	-6
	40	0.99932 +/- 0.00013	0.99996 +/- 0.00010	64	39.585	39.675	17
	70	0.99966 +/- 0.00013	1.00011 +/- 0.00026	45	44.714	44.718	0
HGB_70	0	1.00004 +/- 0.00014	0.99993 +/- 0.00010	-11	21.892	21.933	12
	1	0.99992 +/- 0.00013	0.99982 +/- 0.00009	-10	30.236	30.184	-14
	3	0.99969 +/- 0.00013	1.00026 +/- 0.00009	57	32.326	32.456	34
	40	0.99948 +/- 0.00015	1.00059 +/- 0.00009	111	39.630	40.017	72
	70	0.99967 +/- 0.00012	0.99958 +/- 0.00022	-9	44.684	44.355	-40
HTA_70	0	1.00010 +/- 0.00013	1.00009 +/- 0.00010	-1	24.279	24.209	-21
	1	0.99972 +/- 0.00015	1.00010 +/- 0.00010	38	32.873	32.955	21
	3	0.99914 +/- 0.00012	0.99954 +/- 0.00010	40	35.141	35.171	7
	40	0.99976 +/- 0.00011	0.99994 +/- 0.00009	18	44.379	44.048	-42
	70	0.99940 +/- 0.00014	0.99997 +/- 0.00035	57	51.164	50.800	-5
HTB_70	0	1.00038 +/- 0.00013	0.99983 +/- 0.00010	-55	24.392	24.278	-34
	1	0.99983 +/- 0.00014	1.00022 +/- 0.00009	39	32.946	33.124	45
	3	1.00009 +/- 0.00013	1.00037 +/- 0.00010	28	35.790	35.599	-44
	40	0.99997 +/- 0.00013	0.99983 +/- 0.00009	-14	44.683	44.158	-65
	70	0.99963 +/- 0.00014	0.99968 +/- 0.00019	5	51.918	51.617	1
HWA_70	0	1.00009 +/- 0.00015	1.00024 +/- 0.00010	15	21.578	21.605	8
	1	0.99967 +/- 0.00015	0.99995 +/- 0.00010	28	29.793	29.813	5
	3	0.99959 +/- 0.00013	1.00027 +/- 0.00009	68	32.062	32.168	28
	40	0.99965 +/- 0.00013	1.00044 +/- 0.00010	79	39.384	39.505	23
	70	0.99995 +/- 0.00012	1.00023 +/- 0.00019	28	44.583	44.577	-1
HWB_70	0	1.00008 +/- 0.00013	0.99971 +/- 0.00010	-37	20.713	20.616	-29
	1	0.99986 +/- 0.00015	0.99999 +/- 0.00009	13	28.948	28.930	-5
	3	0.99930 +/- 0.00013	0.99994 +/- 0.00010	64	30.963	31.044	22
	40	0.99953 +/- 0.00015	1.00005 +/- 0.00010	52	37.979	38.036	12
	70	0.99941 +/- 0.00014	1.00008 +/- 0.00027	67	42.306	42.164	-22

Table 12: Integral Neutron Flux, Cumulative Fission Density and Xe-135 and Sm-149 Inventories Comparison for Fresh HEU Core / 70-day Cycle

Case ID	Result Type	MCODE – ADDER Difference	Element	Plate	Axial Node
H0_70	Integral Neutron Flux	-9.74%	C-9	1	3
	Cumulative Fission Density	-2.797 x 10^{19} fis/cm^3	C-4	1	4
	Xe-135	-14.77%	C-14	1	3
	Sm-149	-3.44%	C-15	1	2
HFA_70	Integral Neutron Flux	-8.19%	C-4	1	4
	Cumulative Fission Density	-2.290 x 10^{19} fis/cm^3	C-9	1	4
	Xe-135	-11.74%	C-9	1	3
	Sm-149	3.26%	C-13	9	10
HFB_70	Integral Neutron Flux	-9.22%	C-4	1	4
	Cumulative Fission Density	-2.347 x 10^{19} fis/cm^3	C-14	1	4
	Xe-135	-13.13%	C-14	1	4
	Sm-149	-3.99%	C-9	1	1
HGA_70	Integral Neutron Flux	-9.64%	C-14	1	4
	Cumulative Fission Density	-2.581 x 10^{19} fis/cm^3	C-4	1	4
	Xe-135	-13.17%	C-4	1	3
	Sm-149	3.22%	C-2	15	4
HGB_70	Integral Neutron Flux	-8.89%	C-9	1	4
	Cumulative Fission Density	-2.428 x 10^{19} fis/cm^3	C-4	1	4
	Xe-135	-13.60%	C-9	1	3
	Sm-149	3.37%	B-1	3	5
HTA_70	Integral Neutron Flux	-13.27%	C-4	1	2
	Cumulative Fission Density	-2.910 x 10^{19} fis/cm^3	C-14	1	3
	Xe-135	**-21.51%**	**C-14**	**1**	**2**
	Sm-149	-5.35%	C-15	1	1
HTB_70	**Integral Neutron Flux**	**-13.80%**	**C-9**	**1**	**2**
	Cumulative Fission Density	-3.157 x 10^{19} fis/cm^3	C-14	1	3
	Xe-135	-20.86%	C-14	1	2
	Sm-149	**-6.99%**	**C-15**	**1**	**2**
HWA_70	Integral Neutron Flux	-9.65%	C-4	1	4
	Cumulative Fission Density	-2.407 x 10^{19} fis/cm^3	C-14	1	4
	Xe-135	-14.18%	C-14	1	3
	Sm-149	-3.51%	C-15	1	3
HWB_70	Integral Neutron Flux	-8.00%	C-4	1	4
	Cumulative Fission Density	**-3.186 x 10^{19} fis/cm^3**	**C-9**	**1**	**5**
	Xe-135	-11.82%	C-14	1	4
	Sm-149	3.17%	B-8	11	14

The highest EOC integral neutron flux difference (-13.80%) is reached by case HTB in fuel element C-9, plate 1 and axial node 2. For H0 ADDER results at EOC, the average MCNP flux uncertainty is 0.29% and the maximum MCNP flux uncertainty is 0.52%.

The highest EOC cumulative fission density difference (-3.186 x 10^{19} fis/cm^3) is reached by case HWB in fuel element C-9, plate 1 and axial node 5. This value is above the acceptable uncertainty during fuel management described in 3.3.2 (~1.8 x 10^{19} fis/cm^3), while remaining of the same order of magnitude. The highest difference between MCODE and ADDER results for this metric should be reassessed at the end of a 10-cycle calculation, to measure the impact of fuel management (shuffling, rotation, flipping) on end-of-life cumulative fission density differences.

The highest EOC Xe-135 inventory difference (-21.51%) is reached by case HTA in fuel element C-14, plate 1 and axial node 2. The highest EOC Sm-149 inventory difference (-6.99%) is reached by case HTB in fuel element C-15, plate 1 and axial node 2.

Most peak differences are located in C-ring fuel elements and top axial nodes, which are closer to the shim blades (see Figure 2).

Using the visualization scripts described in 4.3.2, the spatial dependency of MCODE-ADDER integral neutron flux differences are plotted both on a MITR core map and for each fuel element for case H0 at EOC (see Figures 17 and 18). The presented fuel elements are A-2, B-1 and C-9 to represent each ring (C-9 being the element where the highest local difference is located). These figures confirm the fact that the highest differences are located near the shim blades at EOC, which are inserted down to axial node 4 for a withdrawal equal to 46.056 cm (MCODE) or 45.395 cm (ADDER).

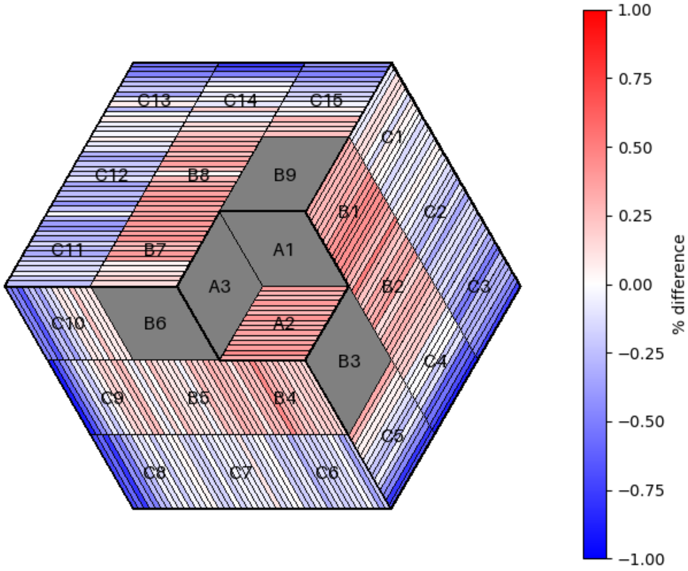


Figure 17: Integral Neutron Flux Core Comparison for case H0_70 EOC

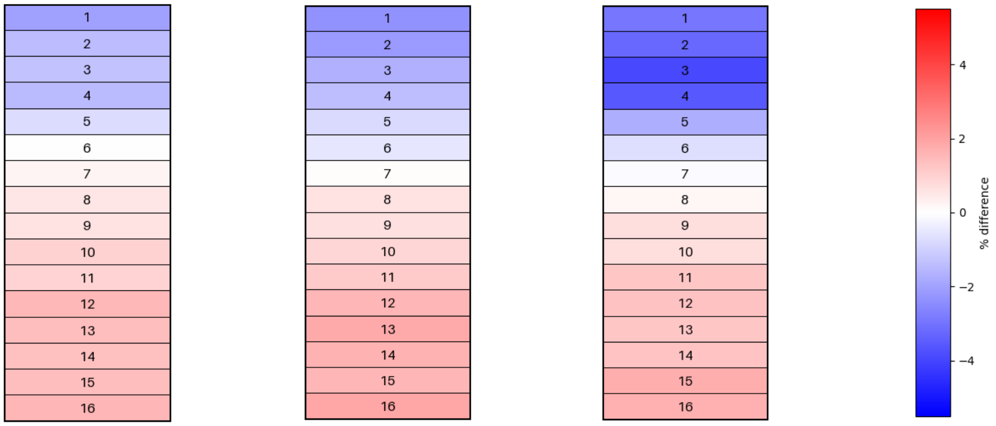


Figure 18: Integral Neutron Flux Fuel Elements Comparison for case H0_70 EOC (A-2, B-1 and C-9)

The integral neutron flux differences are also plotted for case H0 at BOC (first depletion step one-group flux), and the fuel element plots confirm that the highest differences are located near shim blades, which are halfway inserted at BOC (see Figure 19).

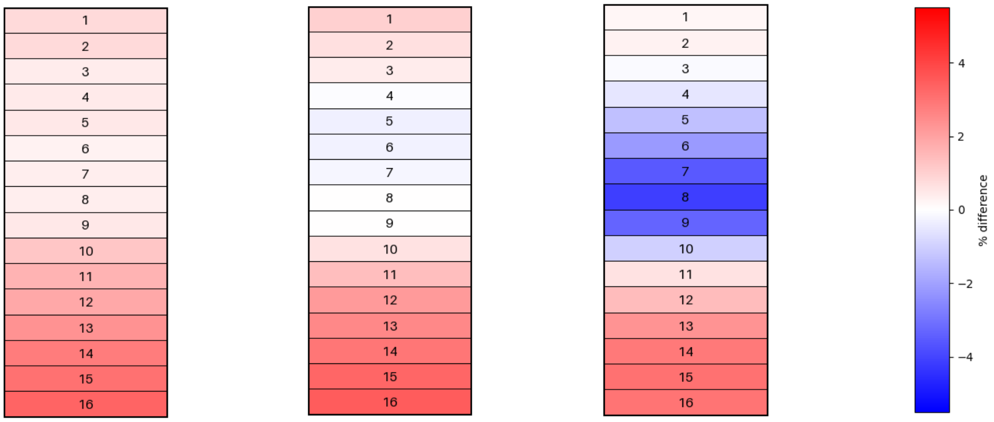


Figure 19: Integral Neutron Flux Fuel Elements Comparison for case H0_70 BOC (A-2, B-1 and C-9)

Case H0 was rerun while forcing ADDER shim bank heights to be the same as MCODE-computed ones to assess the impact of these differences on results. The results are similar to the original case. The critical search algorithm is therefore not identified as a major contribution to the differences located near the shim blades.

In the previous comparisons, the one-group neutron fluxes used for depletion are computed differently by MCODE and ADDER because the predictor-corrector methods are different. The analyzed neutron flux for MCODE is the average between the predictor flux and the corrector flux which is computed after the MCNP model is updated with end of step compositions (cf. 2.3.1.1). Moreover, as described in [16], it is possible that MCODE-FM carries out a critical search before computing the corrector flux, which adds to the differences between the two predictor-corrector schemes.

Case H0 was therefore rerun with the predictor-only method for both MCODE and ADDER to assess the impact of the difference in depletion methods on results. The BOC results are presented in Figures 20 and 21, and the EOC results are presented in Figures 22 and 23. EOC Xe-135 concentrations are also presented in Figures 24 and 25.

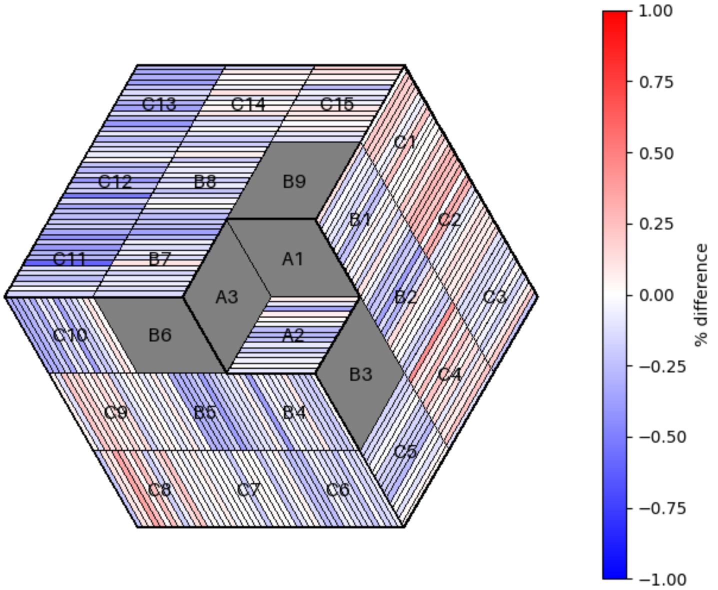


Figure 20: Integral Neutron Flux Core Comparison for case H0_70 BOC (Predictor Only)

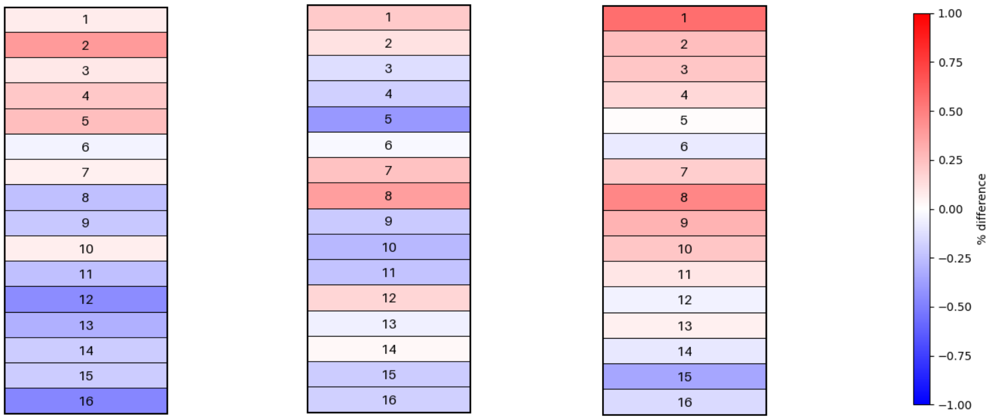


Figure 21: Integral Neutron Flux Fuel Elements Comparison for case H0_70 BOC (A-2, B-1 and C-4, Predictor Only)

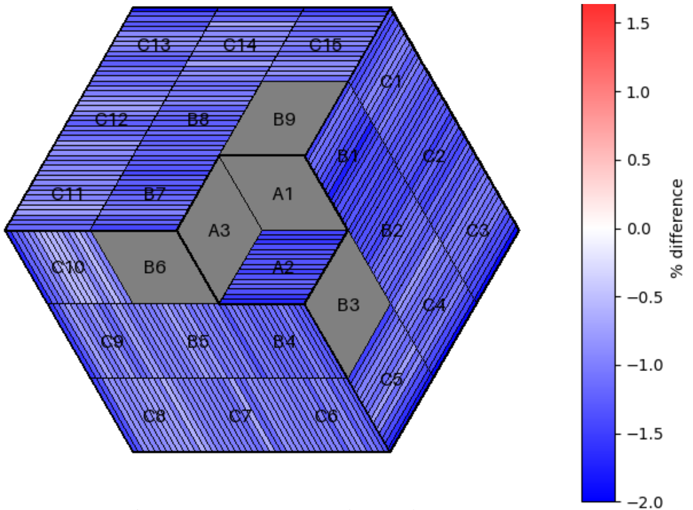


Figure 22: Integral Neutron Flux Core Comparison for case H0_70 EOC (Predictor Only)

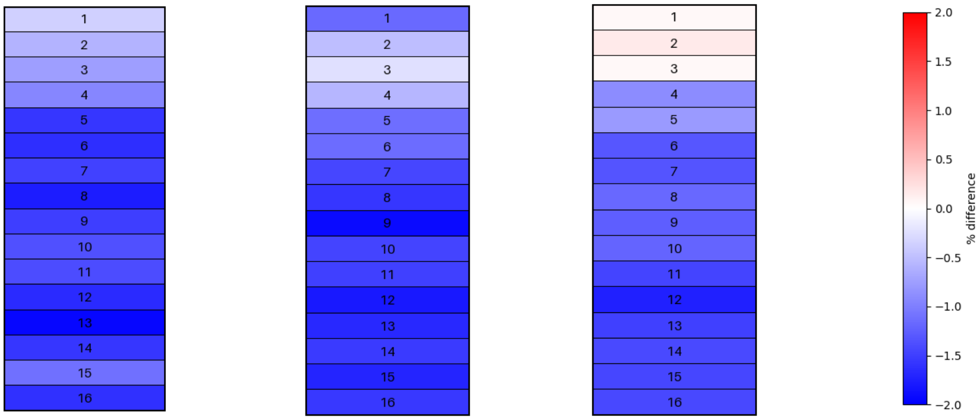


Figure 23: Integral Neutron Flux Fuel Elements Comparison for case H0_70 EOC (A-2, B-1 and C-4, Predictor Only)

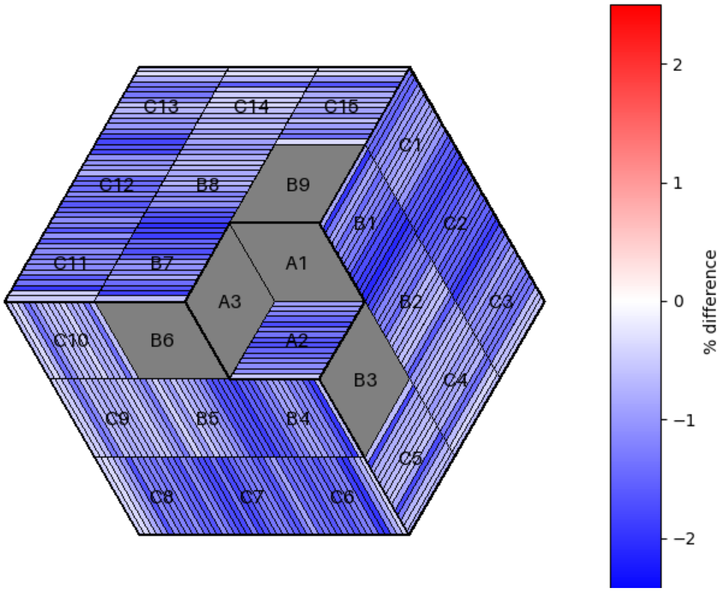


Figure 24: Xe-135 Concentration Core Comparison for case H0_70 EOC (Predictor Only)

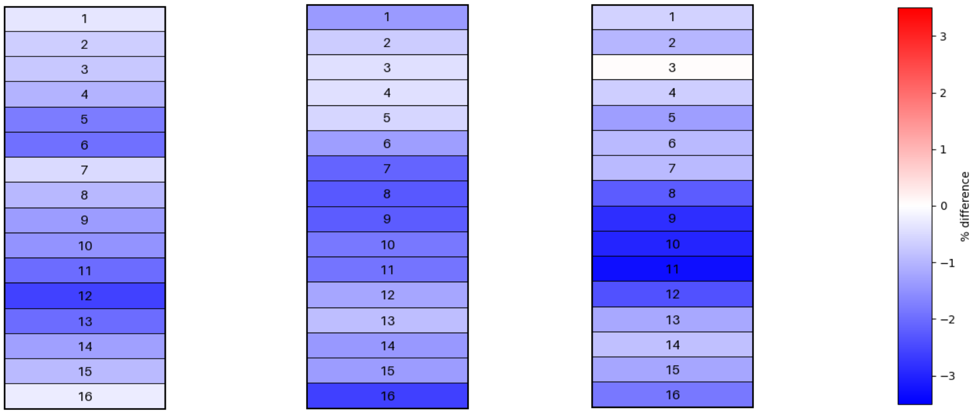


Figure 25: Xe-135 Concentration Fuel Elements Comparison for case H0_70 EOC (A-2, B-1 and C-2, Predictor Only)

As can be seen in Figures 20 to 25, the concentration of high differences in flux near the shim blades cannot be seen anymore when switching to a predictor-only method. BOC results are consistent with the statistical differences that can observed between two separate MCNP calculations carried out with the same model.

EOC results show lower flux and Xe-135 levels for ADDER results, without any local discrepancy near the shim blades. The highest relative difference in integral neutron flux at EOC is equal to -3.54% and reached in element C-4, plate 1 and axial node 15. The highest relative difference Xe-135 at EOC is equal to -4.72% and reached in element C-2, plate 10 and axial node 16.

The evolution of Xe-135 core inventory over time is presented in Figure 26. Lower Xe-135 levels in ADDER results is accompanied by higher U-235 core inventory, the evolution of which over time is shown in Figure 27.

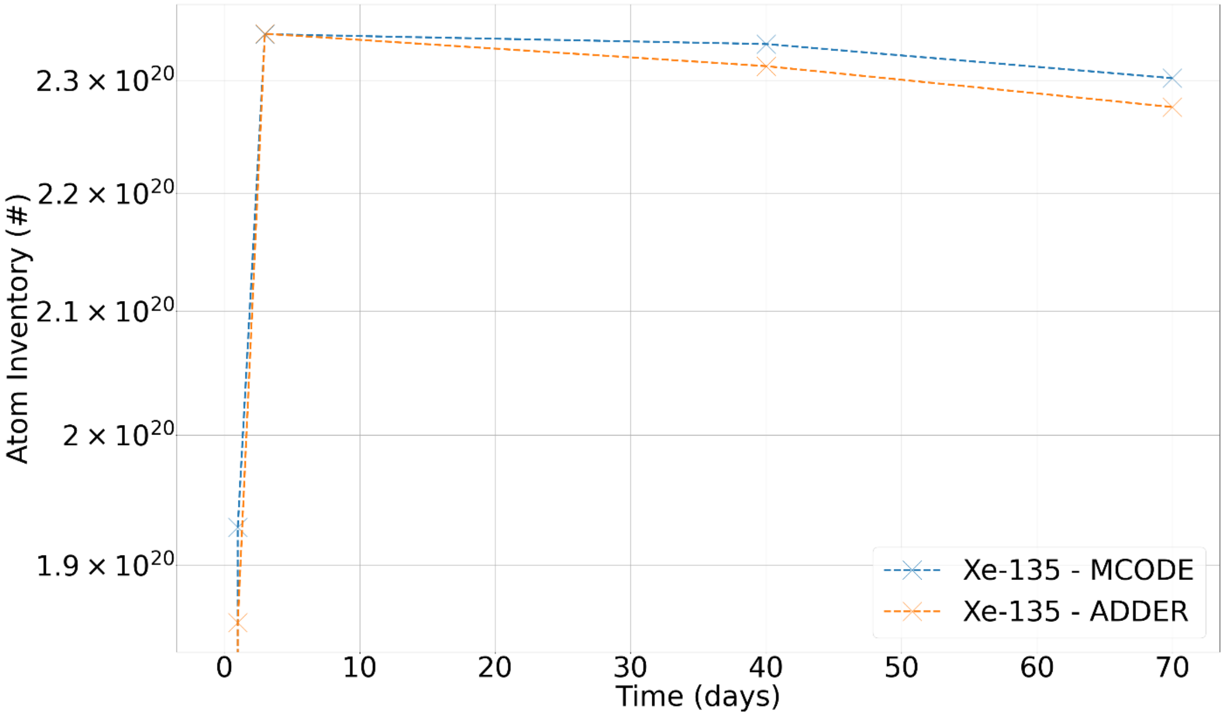


Figure 26: Xe-135 Core Inventory Evolution in ADDER and MCODE results for case H0_70 (Predictor Only)

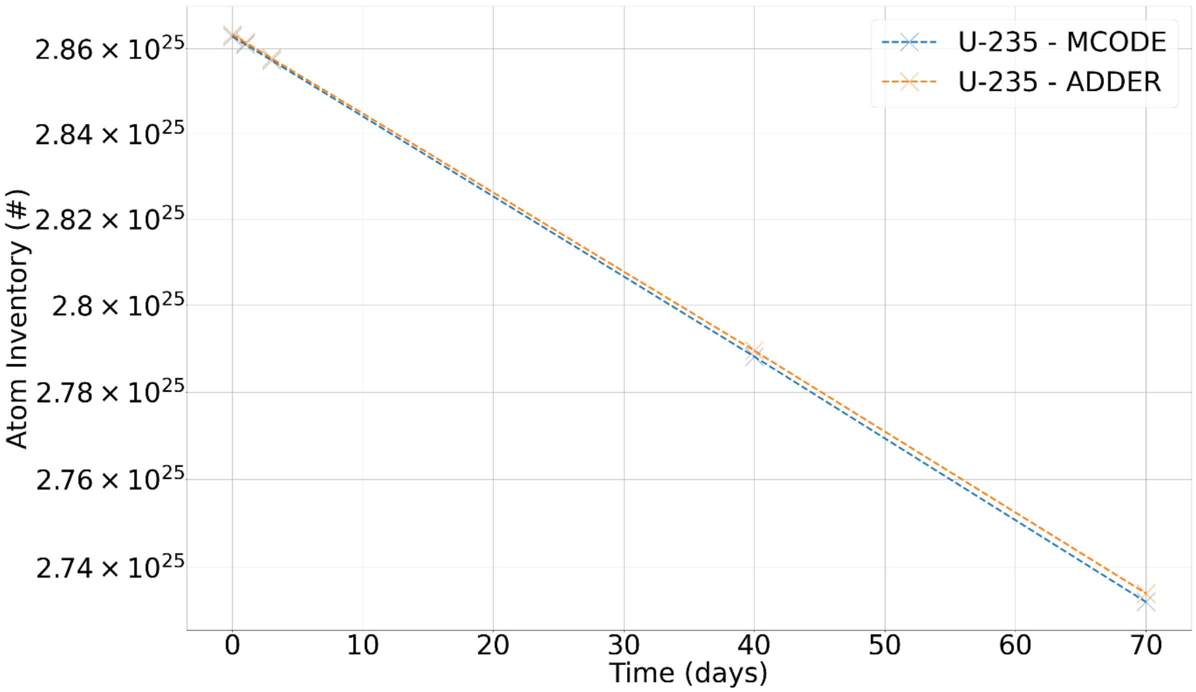


Figure 27: U-235 Core Inventory Evolution in ADDER and MCODE results for case H0_70 (Predictor Only)

The difference in predictor-corrector methods used by MCODE and ADDER is therefore considered to play a major role in the highest differences in neutron flux located near the shim blades. Remaining differences will need to be characterized through further analysis described in 5.2.1, which will include investigation of the way both software handle flux normalization, data libraries and material compositions, as well as the convergence of the selected depletion scheme. Ideally, a comparison should be made using a tightly converged simulation on very fine time steps to properly compare the two software.

As described in 3.2.2, the main tracked actinide for MITR fuel management is U-235, with an acceptable uncertainty of ~0.5 g per fuel element at EOC for HEU cases. U-236, Pu-239 and Np-237 are also of interest for MITR operators. For each HEU case, Table 13 presents the fuel elements which presents the highest difference in each of these four actinides mass.

The highest EOC U-235 mass difference (0.2993 g, relative difference of 0.062%) is reached by case HWA in fuel element C-8. This value is below the acceptable uncertainty of ~0.5 g.

The highest EOC U-236 mass difference (6.054×10^{-2} g, relative difference of 0.854%) is reached by case HTB in fuel element A-2, the highest EOC Pu-239 mass difference (2.269×10^{-3} g, relative difference of 1.065%) is reached by case HTA in fuel element A-2 and the highest EOC Np-237 mass difference (1.257×10^{-3} g, relative difference of 3.456%) is reached by case HTB in fuel element B-7.

Table 13: Major Actinides Mass Comparison for Fresh HEU Core / 70-day Cycle

Case ID	Result Type	MCODE – ADDER Difference (g)	Element
H0_70	U-235	2.487E-1	C-8
	U-236	5.477E-2	A-2
	Pu-239	2.123E-3	B-7
	Np-237	8.778E-4	B-1
HFA_70	U-235	2.315E-1	C-13
	U-236	4.384E-2	A-2
	Pu-239	1.929E-3	A-2
	Np-237	9.134E-4	B-7
HFB_70	U-235	2.555E-1	C-13
	U-236	5.176E-2	A-2
	Pu-239	1.464E-3	C-6
	Np-237	9.151E-4	A-2
HGA_70	U-235	2.641E-1	C-3
	U-236	5.513E-2	A-2
	Pu-239	2.223E-3	C-14
	Np-237	9.298E-4	B-1
HGB_70	U-235	2.567E-1	C-13
	U-236	5.075E-2	A-2
	Pu-239	1.875E-3	A-2
	Np-237	9.244E-4	B-1
HTA_70	U-235	2.503E-1	C-8
	U-236	5.356E-2	B-4
	Pu-239	**2.269E-3**	**A-2**
	Np-237	8.878E-4	B-7
HTB_70	U-235	2.659E-1	C-8
	U-236	**6.054E-2**	**A-2**
	Pu-239	1.956E-3	A-2
	Np-237	**1.257E-3**	**B-7**
HWA_70	**U-235**	**2.993E-1**	**C-8**
	U-236	5.610E-2	A-2
	Pu-239	1.635E-3	B-2
	Np-237	1.039E-3	B-1
HWB_70	U-235	2.634E-1	C-8
	U-236	5.238E-2	A-2
	Pu-239	1.973E-3	A-2
	Np-237	1.074E-3	A-2

4.5.2. Fresh LEU Core Results

The fresh LEU core configuration used for this analysis is described in 3.1.2.

4.5.2.1. Global Results

Shim bank heights and k_{eff} results of the 70-day cycle ADDER and MCODE calculations are presented in Table 14. Shim bank height differences are converted to worth differences by using the LEU shim bank worth presented in 4.1.3.

MCODE and ADDER k_{eff} results are always within 200 pcm of each other thanks to the ± 100 pcm tolerance set for critical searches (cf. Chapter 2). For ADDER calculations, the number of simulated neutrons is adapted during the critical search to optimize the calculation duration, leading to higher standard deviations (compared with MCODE). After the search, a new MCNP calculation is carried out by ADDER with the adequate shim bank height to compute fluxes and reaction rates used for depletion (predictor step), with the user-specified kcode card. Such MCNP calculations have lower standard deviations, closer to MCODE ones (~10 pcm). Their k_{eff} and standard deviations are presented in Table 11, except for the end of cycle, for which the last results of the critical search are presented because this search is not followed by a depletion calculation.

MCODE and ADDER shim bank height results are also within 200 pcm of each other, and do not increase after each depletion step, which shows good agreement between the two software for this metric, for all types and positions of ICE. The highest worth difference (99 pcm) is attained for case LFB at day 40.

4.5.2.2. Local Results

The maximum difference and its location (element / plate / axial node) are presented in Table 14 for the different result types for fresh LEU cases at EOC. The results are presented in the same way as in Table 12.

The highest EOC integral neutron flux difference (-13.21%) is reached by case LTA in fuel element C9, plate 1, axial node 3 and lateral node 3. For L0 ADDER results at EOC, the average MCNP flux uncertainty is 0.56% and the maximum MCNP flux uncertainty is 1.13%. The uncertainties are higher than for the HEU case because the LEU MCNP model fuel cells are smaller (lateral segmentation).

The highest EOC cumulative fission density difference (1.328×10^{20} fis/cm^3) is reached by case LTB in fuel element C3, plate 17, axial node 13 and lateral node 1. The acceptable uncertainty on cumulative fission densities described for HEU cases cannot be applied as is to the LEU results, because the size of the nodes is different due to lateral segmentation, and because the expected fission densities in LEU plates are different than for HEU plates (see Table 2).

The highest EOC Xe-135 (-22.66%) and Sm-149 (-9.91%) inventory differences are reached by case LTA in fuel element C14, plate 1, axial node 2 and lateral node 1.

LEU peak differences are of the same order of magnitude as HEU peak differences, except for cumulative fission densities differences, which are higher in LEU cases (cf. Table 12). Most peak differences are located in C-ring fuel elements and top axial nodes, which are closer to the shim blades (see Figure 2), except for cumulative fission density peak differences, which are located at the bottom of B-ring and C-ring fuel elements.

Table 14: k_{eff} and Shim Bank Height Comparison for Fresh LEU Core / 70-day Cycle

Case ID	Day	MCODE k_{eff}	ADDER k_{eff}	k_{eff} Difference (pcm)	MCODE Shim Bank Height (cm)	ADDER Shim Bank Height (cm)	Worth Difference (pcm)
L0_70	0	0.99983 +/- 0.00011	1.00009 +/- 0.00010	26	23.691	23.720	7
	1	1.00013 +/- 0.00012	0.99978 +/- 0.00009	-35	30.630	30.673	10
	3	0.99913 +/- 0.00013	0.99992 +/- 0.00009	79	32.674	33.003	72
	40	0.99947 +/- 0.00013	1.00029 +/- 0.00008	82	39.565	40.078	81
	70	0.99987 +/- 0.00013	1.00049 +/- 0.00020	62	44.754	44.977	22
LFA_70	0	1.00046 +/- 0.00012	1.00017 +/- 0.00009	-29	23.456	23.446	-3
	1	0.99974 +/- 0.00013	1.00003 +/- 0.00010	29	30.261	30.348	20
	3	0.99980 +/- 0.00011	1.00007 +/- 0.00008	27	32.763	32.651	-25
	40	0.99966 +/- 0.00011	1.00015 +/- 0.00009	49	38.970	39.428	76
	70	0.99986 +/- 0.00012	1.00010 +/- 0.00016	24	44.063	44.170	12
LFB_70	0	1.00001 +/- 0.00014	1.00029 +/- 0.00008	28	23.457	23.558	26
	1	0.99986 +/- 0.00012	1.00017 +/- 0.00009	31	30.297	30.446	35
	3	1.00002 +/- 0.00011	1.00033 +/- 0.00009	31	32.835	32.945	24
	40	**0.99927 +/- 0.00012**	**1.00017 +/- 0.00009**	**90**	**38.990**	**39.590**	**99**
	70	0.99947 +/- 0.00012	1.00013 +/- 0.00013	66	43.916	44.494	62
LGA_70	0	0.99976 +/- 0.00014	1.00017 +/- 0.00008	41	23.381	23.447	17
	1	0.99980 +/- 0.00012	1.00010 +/- 0.00008	30	30.226	30.409	43
	3	0.99984 +/- 0.00012	1.00004 +/- 0.00009	20	32.796	32.728	-15
	40	0.99944 +/- 0.00012	0.99935 +/- 0.00009	-9	39.051	38.939	-19
	70	0.99978 +/- 0.00013	1.00021 +/- 0.00020	43	43.776	44.264	54
LGB_70	0	1.00012 +/- 0.00013	1.00046 +/- 0.00010	34	23.427	23.538	29
	1	1.00003 +/- 0.00012	1.00000 +/- 0.00010	-3	30.347	30.353	1
	3	0.99990 +/- 0.00012	1.00034 +/- 0.00008	44	32.722	32.881	35
	40	0.99975 +/- 0.00011	1.00014 +/- 0.00008	39	39.217	39.44	37
	70	0.99941 +/- 0.00012	1.00015 +/- 0.00027	74	43.836	43.92	9
LTA_70	0	1.00008 +/- 0.00013	0.99987 +/- 0.00008	-21	25.496	25.413	-21
	1	0.99981 +/- 0.00014	1.00017 +/- 0.00010	36	32.694	32.949	56
	3	0.99928 +/- 0.00012	1.00029 +/- 0.00009	101	35.338	35.649	62
	40	0.99968 +/- 0.00013	1.00022 +/- 0.00009	54	42.926	43.547	74
	70	0.99944 +/- 0.00010	0.99992 +/- 0.00030	48	49.291	50.004	21
LTB_70	0	1.00015 +/- 0.00015	1.00000 +/- 0.00009	-15	25.516	25.490	-7
	1	0.99942 +/- 0.00011	0.99997 +/- 0.00009	55	32.724	32.868	32
	3	1.00004 +/- 0.00011	1.00026 +/- 0.00009	22	35.600	35.554	-9
	40	0.99958 +/- 0.00013	1.00015 +/- 0.00009	57	42.901	43.518	74
	70	0.99928 +/- 0.00012	1.00005 +/- 0.00018	77	49.207	50.265	29
LWA_70	0	1.00014 +/- 0.00014	0.99998 +/- 0.00009	-16	22.312	22.318	2
	1	1.00007 +/- 0.00014	1.00027 +/- 0.00009	20	29.220	29.336	28
	3	1.00025 +/- 0.00013	1.00009 +/- 0.00008	-16	31.735	31.643	-21
	40	0.99978 +/- 0.00013	1.00015 +/- 0.00009	37	37.806	38.138	59
	70	0.99936 +/- 0.00013	0.99992 +/- 0.00031	56	41.860	42.213	47
LWB_70	0	0.99990 +/- 0.00013	1.00002 +/- 0.00009	12	21.445	21.51	17
	1	0.99996 +/- 0.00013	1.00003 +/- 0.00009	7	28.350	28.352	0
	3	1.00008 +/- 0.00012	0.99994 +/- 0.00009	-14	30.808	30.495	-73
	40	0.99978 +/- 0.00013	0.99976 +/- 0.00008	-2	36.471	36.519	9
	70	0.99949 +/- 0.00012	1.00010 +/- 0.00022	61	40.544	40.893	52

Table 15: Integral Neutron Flux, Cumulative Fission Density and Xe-135 and Sm-149 Inventories Comparison for Fresh LEU Core / 70-day Cycle

Case ID	Result Type	MCODE – ADDER Difference	Element	Plate	Axial Node	Lateral Node
L0_70	Integral Neutron Flux	-9.68%	C-9	1	4	3
	Cumulative Fission Density	9.253 x 10^{19} fis/cm^{3}	C-3	15	15	1
	Xe-135	-19.05%	C-14	1	3	2
	Sm-149	-7.85%	C-7	11	2	4
LFA_70	Integral Neutron Flux	-10.66%	C-9	1	4	3
	Cumulative Fission Density	1.058 x 10^{20} fis/cm^{3}	C-12	11	14	1
	Xe-135	-16.46%	C-15	1	3	3
	Sm-149	-7.73%	C-4	1	1	1
LFB_70	Integral Neutron Flux	-9.72%	C-4	1	4	2
	Cumulative Fission Density	1.168 x 10^{20} fis/cm^{3}	B-4	8	14	4
	Xe-135	-16.23%	C-15	2	3	3
	Sm-149	7.02%	C-2	19	10	1
LGA_70	Integral Neutron Flux	-10.95%	C-9	1	4	3
	Cumulative Fission Density	1.234 x 10^{20} fis/cm^{3}	C-1	2	15	1
	Xe-135	-17.30%	C-4	1	4	3
	Sm-149	6.75%	B-2	4	14	3
LGB_70	Integral Neutron Flux	-11.34%	C-9	1	4	2
	Cumulative Fission Density	8.839 x 10^{19} fis/cm^{3}	C-2	8	14	3
	Xe-135	-16.09%	C-9	1	4	3
	Sm-149	-7.95%	C-13	6	2	3
LTA_70	**Integral Neutron Flux**	**-13.21%**	**C-9**	**1**	**3**	**3**
	Cumulative Fission Density	1.206 x 10^{20} fis/cm^{3}	B-2	18	15	3
	Xe-135	**-22.66%**	**C-14**	**1**	**2**	**1**
	Sm-149	**-9.91%**	**C-14**	**1**	**2**	**1**
LTB_70	Integral Neutron Flux	-11.98%	C-15	1	2	3
	Cumulative Fission Density	**1.328 x 10^{20} fis/cm^{3}**	**C-3**	**17**	**13**	**1**
	Xe-135	-21.04%	C-9	1	2	2
	Sm-149	-9.74%	C-15	1	2	4
LWA_70	Integral Neutron Flux	-9.29%	C-10	1	4	4
	Cumulative Fission Density	6.855 x 10^{19} fis/cm^{3}	C-13	8	15	2
	Xe-135	-14.47%	C-4	1	4	2
	Sm-149	7.50%	C-14	12	16	1
LWB_70	Integral Neutron Flux	-10.10%	C-9	1	5	3
	Cumulative Fission Density	7.684 x 10^{19} fis/cm^{3}	C-12	7	15	3
	Xe-135	-13.82%	C-15	1	4	4
	Sm-149	7.67%	C-13	15	13	2

Using the visualization scripts described in 4.3.2, the spatial dependency of MCODE-ADDER integral neutron flux differences are plotted both on a MITR core map and for each fuel element for case L0 at EOC (see Figures 28 and 29). The presented fuel elements are A-2, B-1 and C-9 to represent each ring (C-9 being the element where the highest local difference is located). These figures present the same spatial dependency of integral neutron flux differences as the HEU case (see Figures 17 and 18). The impact of the predictor-corrector method on the observed differences is therefore assumed to be similar as for the studied H0 case (cf. 4.5.1.2).

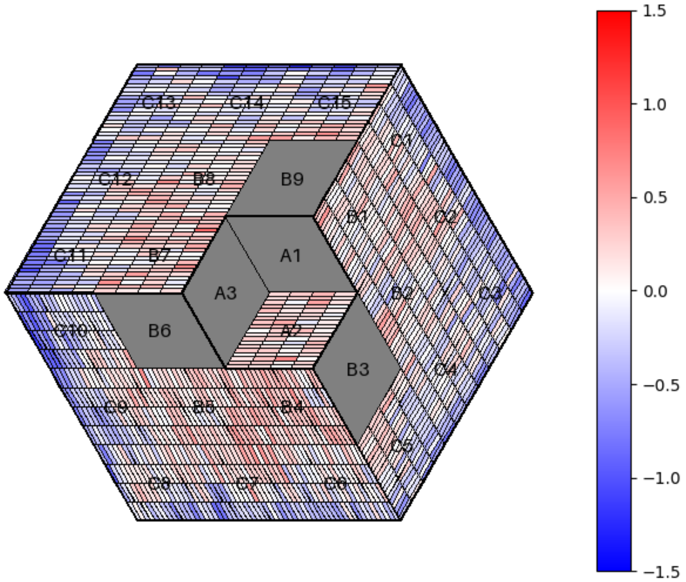


Figure 28: Integral Neutron Flux Core Comparison for case L0_70 EOC

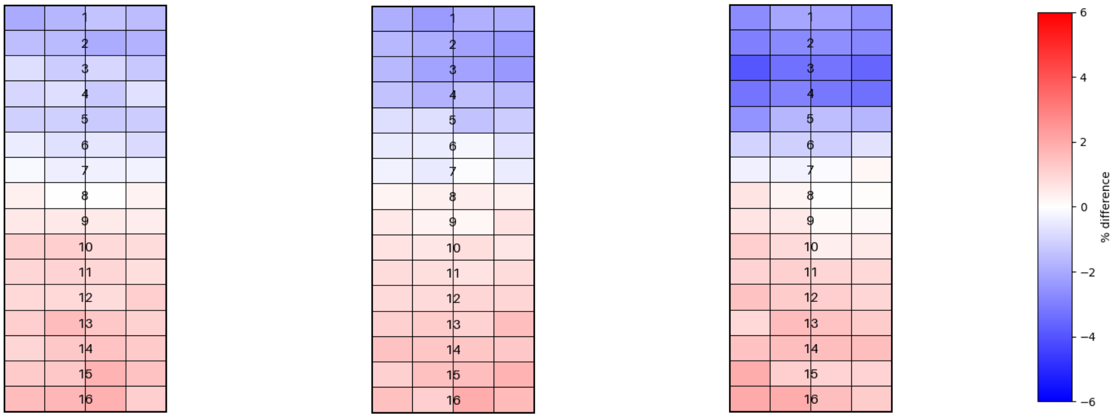


Figure 29: Integral Neutron Flux Fuel Elements Comparison for case L0_70 EOC
(A-2, B-1 and C-9)

As described in 3.2.2, the main tracked actinide for MITR fuel management is U-235. U-236, Pu-239 and Np-237 are also of interest for MITR operators. For each LEU case, Table 16 presents the fuel elements which presents the highest difference in each of these four actinides mass.

The highest EOC U-235 mass difference (0.3062 g, relative difference of 0.039%) is reached by case LWA in fuel element C-3. The highest EOC U-236 mass difference (6.752 x 10^{-2} g, relative difference of 0.275%) is reached by case LWB in fuel element A-2, the highest EOC Pu-239 mass difference (-2.902 x 10^{-2} g, relative difference of -0.754%) is reached by case LGB in fuel element B-4 and the highest EOC Np-237 mass difference (0.4159 x 10^{-3} g, relative difference of 2.522%) is reached by case LGA in fuel element B-7.

These peak differences are similar to the HEU peak differences (cf. Table 13), except for Pu-239 mass. This is consistent with the higher U-238 inventory in fresh LEU fuel elements, which should result in higher Pu-239 concentrations during irradiation in the MITR.

Table 16: Major Actinides Mass Comparison for Fresh LEU Core / 70-day Cycle

Case ID	Result Type	MCODE – ADDER Difference (g)	Element
L0_70	U-235	2.611E-1	C-10
	U-236	5.794E-2	A-2
	Pu-239	-2.458E-2	C-7
	Np-237	1.771E-3	B-5
LFA_70	U-235	2.776E-1	C-8
	U-236	5.549E-2	A-2
	Pu-239	-2.664E-2	C-11
	Np-237	2.643E-3	B-5
LFB_70	U-235	3.059E-1	C-8
	U-236	5.597E-2	A-2
	Pu-239	-2.610E-2	C-2
	Np-237	2.725E-3	B-1
LGA_70	U-235	3.035E-1	C-8
	U-236	6.455E-2	A-2
	Pu-239	-2.748E-2	C-12
	Np-237	**4.159E-3**	**B-7**
LGB_70	U-235	2.762E-1	C-13
	U-236	5.958E-2	A-2
	Pu-239	**-2.902E-2**	**B-4**
	Np-237	2.669E-3	A-2
LTA_70	U-235	2.762E-1	C-8
	U-236	5.537E-2	A-2
	Pu-239	-2.609E-2	C-12
	Np-237	2.114E-3	B-1
LTB_70	U-235	2.943E-1	C-8
	U-236	6.424E-2	A-2
	Pu-239	-2.440E-2	C-7
	Np-237	3.084E-3	B-1
LWA_70	**U-235**	**3.062E-1**	**C-3**
	U-236	6.028E-2	A-2
	Pu-239	-2.740E-2	C-12
	Np-237	2.347E-3	B-7
LWB_70	U-235	3.031E-1	C-13
	U-236	**6.752E-2**	**A-2**
	Pu-239	-2.017E-2	C-7
	Np-237	3.183E-3	B-4

4.6. Full Cycle at Full Power with Mid-Cycle Restart

The cycle modelled with a mid-cycle restart is described in 3.2.3. The result analysis will focus on shim bank heights and Xe-135 inventory, which are the main points of focus in case of a reactor shutdown and restart.

Given their large number of depletion steps and critical searches (cf. Appendix A), calculations with a mid-cycle restart are significantly longer than the previously described calculations. To reduce the number of runs to carry out, this study will focus on MITR cores without any ICEs and with ICEs in position A-1, as no significant differences in results were observed between cores with ICEs in positions A-1 and B-3 in the previous calculations.

4.6.1. Fresh HEU Core Results

Only the highest shim bank worth differences are presented for each HEU calculation with a mid-cycle restart in Table 17. Shim bank height differences are converted to worth differences by using the HEU shim bank worth presented in 4.1.2.

Table 17: Shim Bank Height Comparison for Fresh HEU Core / Mid-cycle Restart (σ~13 pcm)

Case ID	Day / hour / minute	MCODE Shim Bank Height (cm)	ADDER Shim Bank Height (cm)	Worth Difference (pcm)
H0_restart	08:07:00	33.280	32.965	-79
HFA_restart	07:05:30	36.971	36.478	-109
HGA_restart	01:00:00	30.632	30.297	-91
HTA_restart	07:02:30	39.225	38.707	-102
HWA_restart	**07:00:00**	**32.990**	**32.532**	**-117**

MCODE and ADDER shim bank height results are within 200 pcm of each other. Moreover, the highest shim bank worth difference is not reached at the end of the calculation, showing that these differences do not increase after each depletion step. This shows good agreement between the two software for this metric, for all types of ICE in position A-1. The highest worth difference (-117 pcm) is attained for case HWA at day 7.

Xe-135 core inventories in MCODE and ADDER results are compared for case H0_restart after 7 days (before low power period), after 7 days and 7 hours (after low power period) and after 14 days and 7 hours (end of calculation). The results are presented in Table 18.

Table 18: Xe-135 Core Inventory Comparison for Case H0_restart

Day / hour / minute	MCODE Xe-135 Core Inventory	ADDER Xe-135 Core Inventory	Relative Difference in Xe-135 Core Inventory (%)
07:00:00	2.339994E+20	2.339378E+20	-2.63E-02
07:07:00	**2.852910E+20**	**2.851076E+20**	**-6.43E-02**
14:07:00	2.334589E+20	2.334272E+20	-1.36E-02

The compared Xe-135 core inventories for selected times show good agreement between MCODE and ADDER results, with relative differences remaining below 0.1%. Similarly to the results analyzed in 4.5.1.2, Xe-135 inventories in ADDER results are lower than in MCODE results.

4.6.2. Fresh LEU Core Results

Only the highest shim bank worth differences are presented for each LEU calculation with a mid-cycle restart in Table 19. Shim bank height differences are converted to worth differences by using the LEU shim bank worth presented in 4.1.3.

Table 19: Shim Bank Height Comparison for Fresh LEU Core / Mid-cycle Restart (σ~13 pcm)

Case ID	Day / hour / minute	MCODE Shim Bank Height (cm)	ADDER Shim Bank Height (cm)	Worth Difference (pcm)
L0_restart	**07:02:30**	**34.690**	**35.288**	**121**
LFA_restart	07:02:00	34.205	34.567	75
LWA_restart	07:04:30	33.562	33.960	85

MCODE and ADDER shim bank height results are within 200 pcm of each other. Moreover, the highest shim bank worth difference is not reached at the end of the calculation, showing that these differences do not increase after each depletion step. This shows good agreement between the two software for this metric, for FLiBe and pressurized water ICE in position A-1. The highest worth difference (121 pcm) is attained for case HWA after 7 days, 2 hours and 30 minutes (during the low power period).

Xe-135 core inventories in MCODE and ADDER results are compared for case L0_restart after 7 days (before low power period), after 7 days and 7 hours (after low power period) and after 14 days and 7 hours (end of calculation). The results are presented in Table 20.

Table 20: Xe-135 Core Inventory Comparison for Case L0_restart

Day / hour / minute	MCODE Xe-135 Core Inventory	ADDER Xe-135 Core Inventory	Relative Difference in Xe-135 Core Inventory (%)
07:00:00	**3.896176E+20**	**3.867042E+20**	**-7.48E-01**
07:07:00	4.106260E+20	4.095753E+20	-2.56E-01
14:07:00	3.895234E+20	3.869920E+20	-6.50E-01

The compared Xe-135 core inventories for selected times show good agreement between MCODE and ADDER results, with relative differences remaining below 1%. Similarly to the results analyzed for the HEU case, Xe-135 inventories in ADDER results are lower than in MCODE results.

4.7. Optimization of the ADDER Critical Search for the MITR Fuel Management

ADDER critical searches allow the user to specify the range that the shim bank height must belong to. In the previous calculations, this range was set at $[12.70, 53.34]$ (cm) (cf. 2.3.2). However, the approximate height for each step is known thanks to MCODE calculations and, for fuel management, the shim bank height throughout the previous cycle to model is known thanks to operational logs, and the approximate shim bank height can be estimated by looking at previous cycles which are expected to be similar to the next one.

Using MCODE shim bank height results, the ADDER HEU and LEU 70-day cycle calculations described previously are rerun by setting the critical search height range at ± 3 cm of MCODE results, to assess the impact of reducing the range on the number of MCNP calculations to carry out before reaching criticality. Tables 21 and 22 compare such number before and after modifying ranges, with the number of calculations per search for MCODE runs as a reference (the critical search is implemented in a MCODE-FM script, cf. 2.3.1.2).

The modification of height ranges allows to bring the number of calculations from ~5 to ~3, which is similar to the behavior that MCODE-FM achieves with the hardcoded initial differential worth (cf. 2.3.1.2). This flexibility that is brought by ADDER to reduce the time needed to carry out critical searches could be included into MITR-specific scripts when transitioning to ADDER for fuel management.

Table 21: Number of MCNP Calculations Comparison for Fresh HEU Core / 70-day Cycle

Case ID	Day	MCODE-FM Number of MCNP Calculations	ADDER Number of MCNP Calculations with Initial Range	ADDER Number of MCNP Calculations with Modified Range
H0_70	0	4	4	3
	1	2	5	3
	3	3	5	4
	40	3	5	5
	70	4	6	4
HFA_70	0	3	4	3
	1	3	5	4
	3	2	5	3
	40	3	5	3
	70	3	5	3
HFB_70	0	3	4	3
	1	3	5	3
	3	2	5	3
	40	3	6	4
	70	3	5	3
HGA_70	0	4	4	3
	1	2	5	4
	3	2	5	3
	40	3	7	3
	70	3	4	5
HGB_70	0	3	4	3
	1	3	5	3
	3	2	5	4
	40	3	5	3
	70	3	5	3
HTA_70	0	3	5	3
	1	2	5	3
	3	2	6	3
	40	4	7	4
	70	4	5	3
HTB_70	0	3	5	3
	1	2	5	3
	3	3	5	3
	40	4	5	4
	70	5	7	3
HWA_70	0	4	4	3
	1	3	5	3
	3	2	5	3
	40	3	5	3
	70	3	4	5
HWB_70	0	4	5	5
	1	3	5	5
	3	2	5	4
	40	3	5	5
	70	3	5	3

Table 22: Number of MCNP Calculations Comparison for Fresh LEU Core / 70-day Cycle

Case ID	Day	MCODE Number of MCNP Calculations	ADDER Number of MCNP Calculations with Initial Range	ADDER Number of MCNP Calculations with Modified Range
L0_70	0	4	8	3
	1	3	5	4
	3	2	5	3
	40	3	5	3
	70	3	4	3
LFA_70	0	4	4	3
	1	3	5	3
	3	3	5	3
	40	3	5	3
	70	3	5	3
LFB_70	0	4	4	3
	1	3	5	3
	3	3	5	3
	40	3	5	3
	70	3	9	3
LGA_70	0	4	4	3
	1	3	5	5
	3	3	5	3
	40	3	6	3
	70	3	4	4
LGB_70	0	4	4	3
	1	3	5	3
	3	3	5	3
	40	3	5	3
	70	3	7	3
LTA_70	0	4	5	3
	1	3	5	3
	3	3	5	3
	40	3	4	4
	70	4	5	3
LTB_70	0	4	5	4
	1	3	5	3
	3	3	5	3
	40	3	5	3
	70	3	5	3
LWA_70	0	4	4	3
	1	3	5	3
	3	3	5	3
	40	3	5	4
	70	3	6	3
LWB_70	0	4	4	3
	1	3	5	4
	3	3	7	3
	40	3	6	3
	70	3	5	3

5. Conclusions and Future Work

5.1. Feasibility Assessment Conclusion

This analysis shows satisfactory agreement between MCODE and ADDER results to pursue transitioning from MCODE to ADDER for MITR fuel management. The highest calculated differences for 70-day HEU and LEU cases are presented in Table 23, and remain low enough to show the potential of transitioning from MCODE to ADDER.

Table 23: Highest ADDER-MCODE Differences for Fresh HEU and LEU Cores / 70-day Cycle

Core Type	Result Type		Highest MCODE – ADDER Difference
Fresh HEU Core	Shim Bank Height	Global	78 pcm
	Integral Neutron Flux	Per node	-13.80%
	Cumulative Fission Density	Per node	-3.186 x 10^{19} fis/cm^{3}
	Xe-135	Per node	-21.51%
	Sm-149	Per node	-6.99%
	U-235	Per element	2.993 x 10^{-1} g
	U-236	Per element	6.054 x 10^{-2} g
	Pu-239	Per element	2.269 x 10^{-3} g
	Np-237	Per element	1.257 x 10^{-3} g
Fresh LEU Core	Shim Bank Height	Global	99 pcm
	Integral Neutron Flux	Per node	-13.21%
	Cumulative Fission Density	Per node	1.328 x 10^{20} fis/cm^{3}
	Xe-135	Per node	-22.66%
	Sm-149	Per node	-9.91%
	U-235	Per element	3.062 x 10^{-1} g
	U-236	Per element	6.752 x 10^{-2} g
	Pu-239	Per element	-2.902 x 10^{-2} g
	Np-237	Per element	4.159 x 10^{-3} g

Using the predictor-corrector method, higher differences between MCODE and ADDER results are observed near the shim blades indicating that further work is needed to understand the cause of these differences. Both codes use a different algorithm for the predictor-corrector, and the critical blade search is not performed at each MCNP calculation in ADDER. After switching to the predictor method, this local phenomenon is not observed anymore. ADDER results now present overall lower neutron flux and Xe-135 levels indicating most likely differences in power normalization that also need further study. Maximum local differences are decreased from -13.80% to -3.54% for neutron flux and from -21.51% to -4.72% for the fresh HEU core without any in-core experiment.

Moreover, calculations with a mid-cycle restart show satisfactory agreement on shim bank height and Xe-135 core inventory between MCODE and ADDER results, with respective highest differences of 121 pcm and 0.748% reached for the L0_restart case.

Overall, the presented results support the adoption of ADDER as the new MITR fuel management software once validation with the actual reactor measurements is performed. Complementary studies described below will need to be carried out to identify causes for the identified differences (predictor-corrector method impact, and lower ADDER neutron flux and Xe-135 levels).

5.2. Future Work Recommendations

5.2.1. MCODE-ADDER Comparison

To complete the feasibility study of adopting ADDER for the MITR fuel management, further analysis is required to characterize the observed differences described in Chapter 4, including the differences in cumulative fission densities for the LEU case given their large magnitude compared to the HEU case. This includes investigating the way both software handle power normalization and material compositions, and assessing the convergence of the selected depletion scheme. Shorter timesteps at beginning of cycle might be required to accurately track Xe-135 build-up for the studied MITR configurations. This investigation could be carried out using the predictor method as a first step, and differences in predictor-corrector iteration schemes could then be analyzed.

Moreover, cases representative of the current state of MITR need to be studied, to assess the feasibility of adopting ADDER before conversion to LEU. The MITR HEU equilibrium core consists of 24 fuel elements and 3 dummy elements, and its successive core descriptions (fuel element positions, material compositions) are stored as part of the MITR fuel management.

Finally, calculations spanning over multiple cycles would need to be carried out, to compare the fuel management capabilities of both software (shuffle, flip, rotation). Some scripts of MCODE-FM (including *susb.py*) would need to be modified, to accurately rotate plates with lateral segmentation (LEU core model).

The scripts developed during this study to extract data from MCODE and ADDER results and to visualize their differences could be reused for this future work (cf. 4.3).

5.2.2. ADDER Improvement

The current version of ADDER already allows the user to specify different options for critical searches, including height range and critical height guess. Another option that the user could specify for critical searches is the confidence level to be taken into account to assess criticality. Currently, it is set at $\pm 2\sigma$ by ADDER, but adding it as a user-defined option for critical search operations (with a default value to 2σ) could increase the flexibility depending on the user's needs. An easy workaround consists in adjusting the tolerance depending on the expected value of σ.

Xe-135 build-up has a significant impact on depletion calculations at the beginning of a cycle because of its short half-life and large negative reactivity effect. For a reactor that has known operational characteristics, Xe-135 build-up is usually predictable through operational experience. The ability to specify equilibrium Xe-135 levels may allow to skip some beginning of cycle depletion steps, and could be implemented in ADDER.

Another capability that could be useful to ADDER users is the automatic refinement of depletion timesteps if the observed change in a specific quantity (control blades height, Xe-135 inventory...) is too high. However, this would require further evaluation to include this feature in ADDER in a way that is not reactor design-specific.

5.2.3. MCODE to ADDER Transition

Transitioning from MCODE to ADDER for MITR fuel management calculations would require building a MITR-specific Python wrapper for ADDER, similar to MCODE-FM for MCODE, to facilitate fuel management calculations.

First of all, modelling the depleted MITR core requires to know the material composition of each current HEU fuel elements. The latter have been calculated via MCODE calculations. Conversion of MCODE output files that describe depleted fuel elements to readable ADDER input files would therefore need to be carried out before transitioning to ADDER.

In addition to this initial step, the Python wrapper would need to present similar features as MCODE-FM, while providing a better experience and an increased flexibility for the user. This includes reducing the number of required input files, and allowing to easily modify some options without hardcoding them into the wrapper scripts. Some MCODE-FM capabilities, such as building MCNP models of fuel elements based on material descriptions, could be integrated into the wrapper. Moreover, the analysis presented in 4.7 shows that allowing the user to specify the shim bank height range to reduce critical searches computational time could be a useful capability to include in the wrapper.

Finally, if the wrapper includes data processing capabilities, part of the scripts developed for this study could be reused. For instance, the ability to map ADDER materials to cells and cells to specific locations in the core would be required to efficiently post-process data.

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Appendix A: ADDER and MCODE-FM Inputs

Options and cards added at the beginning of all ADDER input files

```
neutronics_solver = "MCNP"
neutronics_exec = /Codes/LANL/MCNP_CODE/bin/mcnp5
use_depletion_library_xs = False
depletion_substeps = 20
depletion_solver = "origen2.2"
depletion_exec = /Codes/origen22/origen22
depletion_method = "cecm"
depletion_library_name = PWRUE
neutronics_reactivity_threshold = 0.001

[materials]
    [[metadata]]
        [[[list_nondeplete]]] #inspired by the ADDER training MITR presentation (slide 22)
-> added 12, 13, 3333, 81 and removed 610, 620 (LEU specific)
            neutronics_ids = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 13, 30, 31, 3333, 40, 4111,
4112, 4113, 60, 61, 81, 100, 601
            depleting = False
            name = "non_depleting"
[control_groups]
    [[control_blades]] #inspired by the ADDER training MITR presentation (slide 24) + lines
2625-2661 of skeleton_input
        set = 864, 872, 876, 900, 903, 905, 908, 909, 911, 913, 915, 917, 918, 921, 923,
926, 927, 929
        type = surface
        axis = z
```

Fresh HEU core MCODE-FM 7-day cycle

```
fixed True
nCycles 1
time 7.0
power 5700000.0
```

Fresh LEU core MCODE-FM 7-day cycle

```
fixed True
nCycles 1
time 7.0
power 7000000.0
```

Fresh HEU core ADDER 7-day cycle

```
[operations]
    [[state 1]]
        label = "BOC"
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 2]]
        label = "MOC_1st_day"
        [[[deplete]]]
            powers = 5.7
            durations = 1
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 3]]
        label = "MOC_3rd_day"
        [[[deplete]]]
            powers = 5.7
            durations = 2
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 4]]
        label = "EOC"
        [[[deplete]]]
            powers = 5.7
            durations = 4
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
```

Fresh LEU core ADDER 7-day cycle

```
[operations]
    [[state 1]]
        label = "BOC"
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 2]]
        label = "MOC_1st_day"
        [[[deplete]]]
            powers = 7
            durations = 1
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 3]]
        label = "MOC_3rd_day"
        [[[deplete]]]
            powers = 7
            durations = 2
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 4]]
        label = "EOC"
        [[[deplete]]]
            powers = 7
            durations = 4
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
```

Fresh HEU core MCODE-FM 70-day cycle

```
fixed True
nCycles 1
time 70.0
power 5700000.0
```

Fresh LEU core MCODE-FM 70-day cycle

```
fixed True
nCycles 1
time 70.0
power 7000000.0
```

Fresh HEU core ADDER 70-day cycle

```
[operations]
    [[state 1]]
        label = "BOC"
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 2]]
        label = "MOC_1st_day"
        [[[deplete]]]
            powers = 5.7
            durations = 1
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 3]]
        label = "MOC_3rd_day"
        [[[deplete]]]
            powers = 5.7
            durations = 2
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 4]]
        label = "MOC_40th_day"
        [[[deplete]]]
            powers = 5.7
            durations = 37
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 5]]
        label = "EOC"
        [[[deplete]]]
            powers = 5.7
            durations = 30
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
```

Fresh LEU core ADDER 70-day cycle

```
[operations]
    [[state 1]]
        label = "BOC"
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 2]]
        label = "MOC_1st_day"
        [[[deplete]]]
            powers = 7
            durations = 1
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 3]]
        label = "MOC_3rd_day"
        [[[deplete]]]
            powers = 7
            durations = 2
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 4]]
        label = "MOC_40th_day"
        [[[deplete]]]
            powers = 7
            durations = 37
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 5]]
        label = "EOC"
        [[[deplete]]]
            powers = 7
            durations = 30
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
```

Fresh HEU core MCODE-FM 70-day cycle with mid-cycle restart

```
fixed True
nCycles 1
time 7.0 7.29167 14.29167
power 5700000.0 100000.0 5700000.0
```

Fresh LEU core MCODE-FM 70-day cycle with mid-cycle restart

```
fixed True
nCycles 1
time 7.0 7.29167 14.29167
power 7000000.0 100000.0 7000000.0
```

Fresh HEU core ADDER 70-day cycle with mid-cycle restart

(only the first 30-minute step is presented here)

```
[operations]
    [[state 1]]
        label = "BOC"
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 2]]
        label = "Pre_restart_1st_day"
        [[[deplete]]]
            powers = 5.7
            durations = 1
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 3]]
        label = "Pre_restart_3rd_day"
        [[[deplete]]]
            powers = 5.7
            durations = 2
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 4]]
        label = "Pre_restart_7th_day"
        [[[deplete]]]
            powers = 5.7
            durations = 4
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
```

```
 [[state 5]]
   label = "Low_power_period_1"
   [[[deplete]]]
     powers = 0.1
     durations = 0.02083
     execute_endpoint = False
   [[[geometry_search]]]
       group_name = control_blades
       k_target = 1
       bracket_interval = 12.70, 53.34
       target_interval = 0.001
[...]
 [[state 19]]
   label = "Post_restart_1st_day"
   [[[deplete]]]
     powers = 5.7
     durations = 1
     execute_endpoint = False
   [[[geometry_search]]]
       group_name = control_blades
       k_target = 1
       bracket_interval = 12.70, 53.34
       target_interval = 0.001
 [[state 20]]
   label = "Post_restart_3rd_day"
   [[[deplete]]]
     powers = 5.7
     durations = 2
     execute_endpoint = False
   [[[geometry_search]]]
       group_name = control_blades
       k_target = 1
       bracket_interval = 12.70, 53.34
       target_interval = 0.001
 [[state 21]]
   label = "Post_restart_7th_day"
   [[[deplete]]]
     powers = 5.7
     durations = 4
     execute_endpoint = False
   [[[geometry_search]]]
       group_name = control_blades
       k_target = 1
       bracket_interval = 12.70, 53.34
       target_interval = 0.001
```

Fresh LEU core ADDER 70-day cycle with mid-cycle restart
(only the first 30-minute step is presented here)

```
[operations]
    [[state 1]]
        label = "BOC"
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 2]]
        label = "Pre_restart_1st_day"
        [[[deplete]]]
            powers = 7
            durations = 1
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 3]]
        label = "Pre_restart_3rd_day"
        [[[deplete]]]
            powers = 7
            durations = 2
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
    [[state 4]]
        label = "Pre_restart_7th_day"
        [[[deplete]]]
            powers = 7
            durations = 4
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001

    [[state 5]]
        label = "Low_power_period_1"
        [[[deplete]]]
            powers = 0.1
            durations = 0.02083
            execute_endpoint = False
        [[[geometry_search]]]
                group_name = control_blades
                k_target = 1
                bracket_interval = 12.70, 53.34
                target_interval = 0.001
  [...]
```

```
[[state 19]]
    label = "Post_restart_1st_day"
    [[[deplete]]]
        powers = 7
        durations = 1
        execute_endpoint = False
    [[[geometry_search]]]
            group_name = control_blades
            k_target = 1
            bracket_interval = 12.70, 53.34
            target_interval = 0.001
[[state 20]]
    label = "Post_restart_3rd_day"
    [[[deplete]]]
        powers = 7
        durations = 2
        execute_endpoint = False
    [[[geometry_search]]]
            group_name = control_blades
            k_target = 1
            bracket_interval = 12.70, 53.34
            target_interval = 0.001
[[state 21]]
    label = "Post_restart_7th_day"
    [[[deplete]]]
        powers = 7
        durations = 4
        execute_endpoint = False
    [[[geometry_search]]]
            group_name = control_blades
            k_target = 1
            bracket_interval = 12.70, 53.34
            target_interval = 0.001
```