AN IMPROVED MCNP-ORIGEN DEPLETION PROGRAM (MCODE) AND ITS VERIFICATION FOR HIGH-BURNUP APPLICATIONS

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ABSTRACT

A new MCNP-ORIGEN linkage code, MCODE, has been developed at MIT, which combines the continuous-energy Monte Carlo code, MCNP-4C, and the one-group depletion code, ORIGEN2.1, to perform burnup calculations. MCNP is capable of providing the neutron flux and effective one-group cross sections for different MCNP-defined regions. ORIGEN, in turn, carries out multi-nuclide depletion calculations for each region and provides material compositions to update beginning-of-timestep MCNP input. This console program is entirely written in ANSI C (about 3000 lines) and is fully portable under Windows and UNIX environments. Two significant features have been emphasized: 1) easy usability including simplified and centralized user input data, automatic generation of tally materials and tallies, automatic execution of MCNP and ORIGEN, and 2) good functionality including flexible normalization options (either constant flux or constant power), internal burnup corrector (in ORIGEN depletions), and implementation of a burnup predictor-corrector algorithm. Two sample calculations are described to demonstrate MCODE validity for high burnup applications. The first is a benchmark for a 9.75 w/o enriched standard UO_2 PWR lattice under cold conditions. Two state-of-the-art codes, CASMO-4 and HELIOS, are used to compare isotopic compositions as well as eigenvalues. The second is a sample calculation for axially heterogeneous ThO_2 and UO_2 pin cells showing the unique capability of the Monte Carlo approach. Although the two demonstrated cases have simple geometries, more complex lattice configurations have been represented using MCODE for fast reactor core analysis.

1. INTRODUCTION

Due to the steady advances of computer power in recent decades, Monte Carlo based codes are becoming more widely used in routine reactor design calculations. Although they are generally much more computationally-demanding than deterministic methods such as collision probability methods, they provide exact solutions to neutron transport equations given a sufficient number of neutron histories and appropriate neutron cross section libraries. Since the Monte Carlo method is, in principle, a virtual analog to the real world, the capabilities to solve transport problems are unlimited as long as one can model the desired system.

MCNP-4C [1], the latest MCNP version, is a general purpose, generalized geometry, continuous energy, time-dependent, Monte Carlo transport code for neutrons/photons/electrons developed at Los Alamos National Laboratory (LANL). But it only provides a snapshot of the reactor neutrons and cannot do reactor burnup calculations. Therefore, another code, ORIGEN2.1 [2], a one-group depletion and radioactive decay computer code using the matrix exponential method to solve a large system of coupled, linear, first-order ordinary differential equations with constant coefficients, is used to carry out burnup calculations. A linkage program, MCODE (MCNP-ORIGEN DEpltion program), has been developed at MIT to manage data transfer and to couple and run these two codes in a repetitive sequence.

The idea of combining MCNP and ORIGEN dates back to the 1980s. In the beginning, users coupled the two codes in a manual way, i.e., ran MCNP first, copied the output from MCNP and organized it into ORIGEN input format, then ran ORIGEN to update the initial MCNP input and re-ran MCNP, and so on. This approach is only practical for a few timesteps and several nuclides. For routine burnup calculations, however, this approach is not acceptable in terms of user time requirements and the propensity to make errors. A console program is needed to automate running of MCNP and ORIGEN. In the late 1990s, the Idaho National Engineering and Environmental Laboratory (INEEL) distributed the first MCNP/ORIGEN linkage program, MOCUP (MCNP-ORIGEN Coupling Utility Program) [3]. Shortly there after, the Los Alamos National Laboratory (LANL) released their version of an MCNP/ORIGEN coupler, MONTEBURNS [4]. Since then, other coupling programs have appeared in the literature [5, 6].

As a bridge program, MCODE distinguishes itself in two ways. The first is its friendly user interface. The input files are substantially simplified, reducing several inputs to only two input files (MCNP and MCODE input files), with a clearly-specified format. Succinct summaries are appended at the end of the log file. Detailed output data can also be found in the output file. The second is its unique way of coupling MCNP and ORIGEN. A standard predictor-corrector algorithm is implemented in the code, which permits larger timesteps.

As with any code, a verification process is necessary for MCODE. In this paper two sample calculations are presented for high burnup applications. High burnup is a challenge for MCODE because an increased number of important fission products and actinides are needed. The first benchmark is a standard PWR lattice with 9.75 w/o enriched UO_2 fuel under cold conditions. The isotopic compositions from CASMO-4 and HELIOS at 100 MWd/kg are compared with MCODE results. The eigenvalues are also compared as a function of burnup. Both show satisfactory agreement compared to the relevant literature [7]. The second sample calculation is for an innovative design of axially heterogeneous UO_2/ThO_2 pin cells [8], from which some general guidelines are drawn. This special case also shows the importance of using a predictor-corrector algorithm.

2. METHODOLOGY

2.1 OVERVIEW

In routine reactor design burnup calculations, the key issue is to determine the time-dependent fuel material compositions as well as the eigenvalues as a function of burnup. Two basic mechanisms of fuel depletion are under consideration: 1) various neutron reactions such as fissions, neutron captures, etc., and 2) the decay of radioactive isotopes. Once material compositions are known eigenvalues can then be calculated efficiently using MCNP.

Mathematically, the burnup problem can be formulated as follows. For the given nuclear system (such as a lattice pin cell, or an assembly, or even whole core), the entire space can be divided into many zones, such as fuel, cladding, water, etc., with appropriate boundaries. In MCNP-4C each zone is called a cell and is defined by its bounding surfaces. Some of the zones containing actinide isotopes (those with atomic number greater than or equal to 90) are called active cells, in which the fuel compositions are assumed uniform and known at the beginning (t=0). Denote a material vector $\mathbf{X}_i(t)$ as the atom number density for active cell i. Suppose there are n active cells altogether. The objective of the burnup calculation is to obtain a material vector $\mathbf{X}_i$, i = 1, 2, …, n, at specified time T given the operating history of the nuclear system. The depletion process can be described by the following equation [9]:

$$\frac{dX_{ij}}{dt} = \sum_{k=1}^{N_i} l_{k\to j}\lambda_k X_{ik} + \sum_{k=1}^{N_i} f_{k\to j} X_{ik}\int \sigma_k(E)\phi_i(E)dE - \lambda_j X_{ij} - X_{ij}\int \sigma_j(E)\phi_i(E)dE \qquad (1)$$

$$i = 1, 2, \cdots, n; \quad j = 1, 2, \cdots, N_i$$

where X_{ij} = atom number density of nuclide j in cell i
N_i = number of nuclides in cell i
$l_{k\to j}$ = fraction of radioactive disintegrations by nuclide k that lead to formation of nuclide j
λ_k = radioactive decay constant of nuclide k
$f_{k\to j}$ = fraction of neutron absorptions by nuclide k that lead to formation of nuclide j
$\phi_i(E)$ = spatial-average neutron energy spectrum in cell i
$\sigma_k(E)$ = neutron absorption cross section of nuclide k

Therefore, in the framework of MCODE burnup calculations, various reaction rates or one-group cross sections as well as the one-group flux in each active cell should be provided by MCNP. Specifically, the effective one-group cross sections of fission products and actinides in each active cell are needed. For fission products, only neutron capture cross sections are calculated since their principal effect is due to neutron absorption. For actinides, four types of cross sections are considered including capture, fission, $(n,2n)$, and $(n,3n)$ reactions because actinides are important in terms of generating fission source neutrons and evolving into higher-mass actinides. Since there is a limited amount of actinides, it is relatively straightforward to identify representative nuclei. The representation of fission products is, however, an ad hoc process especially for high burnup applications, because numerous fission products are being generated [10]. The fractional neutron importance (absorption) of most individual fission products is small and one needs to consider at least 40 in the usual discharge burnup range (40-60 MWd/kg) for LWRs. For high burnup (say 100MWd/kg), ~100 fission products are needed to account for a reasonably complete neutron

absorption fraction (our chosen 100 fission products account for more than 99% of neutron absorptions). All tallies in MCNP come from track length estimates of cell flux and reaction rates (tally type F4 in MCNP). Generally track length estimates are quite reliable because there are frequently many tracks in a cell compared to the number of collisions, leading to many contributions to this tally.

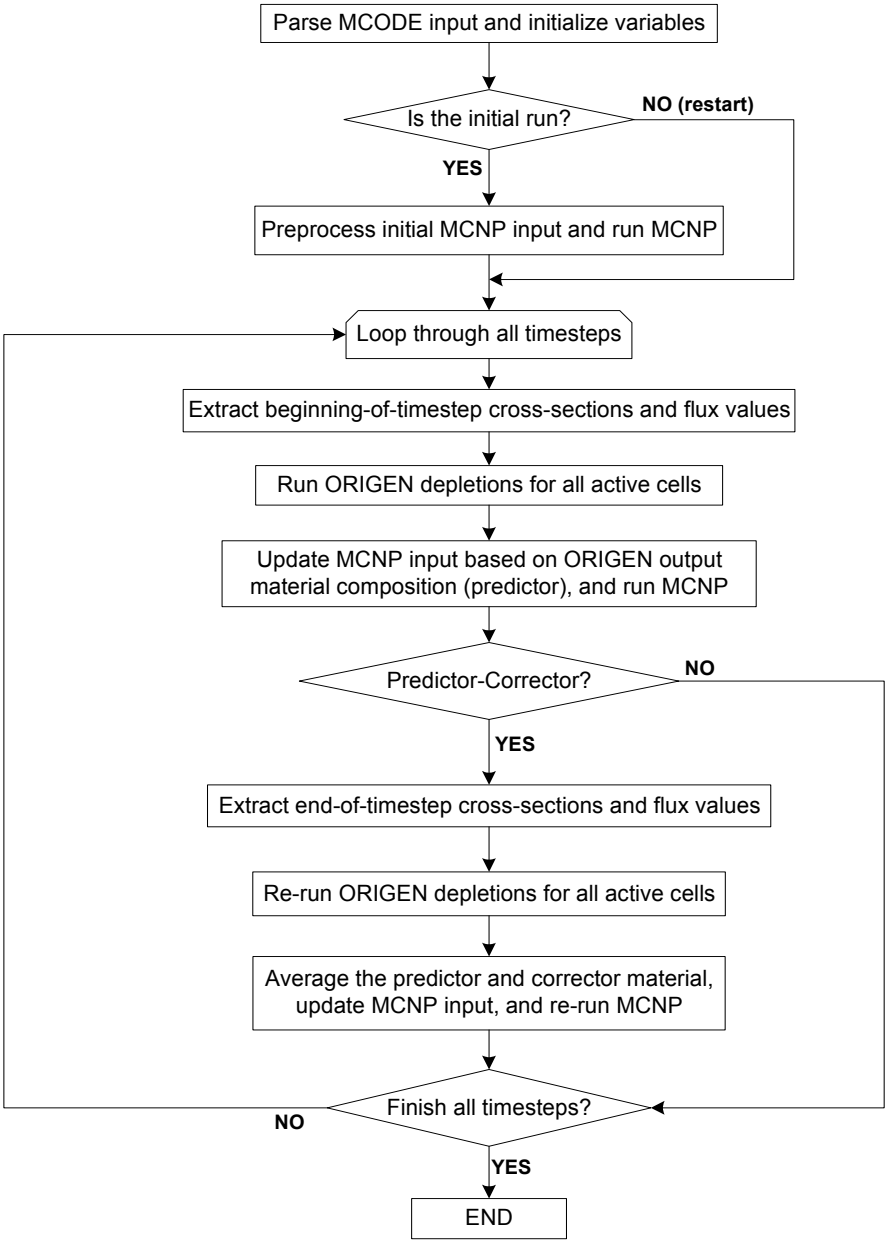

Figure 1. Flow diagram of MCODE.

In order to solve the burnup problem described in Eq. (1), the time T is divided into a number of small time intervals. At the beginning of irradiation, a small timestep size is needed to account for the buildup of steady state xenon concentrations in light water reactors. After ~20 MWd/kg, a larger size

timestep is acceptable, for example, 5 MWd/kg. Assuming constant cross section and flux within each time interval, one can then use the matrix exponential method to solve these small time intervals in a tandem way. Since MCNP only accounts for important isotopes, all other cross sections not provided must use values from ORIGEN one-group cross section libraries, which are fairly good for specific types of reactors and fuels.

The flow of calculations of MCODE is shown in the simplified diagram illustrated in Figure 1. As can be seen, it alternately executes MCNP and ORIGEN to do burnup calculations.

2.2 NORMALIZATION

MCNP generates various one-group cross sections and one-group flux values, using track length estimates, for ORIGEN. The one-group cross section values are in units of barns and ready to use. Since all tallies in MCNP are normalized as per fission source neutron, the flux values are in units of (number-of-neutrons)/(fission-source-neutron)/cm^2, which needs to be multiplied by a constant factor to convert into (number-of-neutrons)/(cm^2·second). The typical way of calculating this flux multiplication factor (FMF) as recommended in the MCNP manual [1] is

$$\mathrm{FMF} = \frac{P \cdot \bar{\nu}}{Q \cdot k_{\mathrm{eff}}} \tag{2}$$

where P = total power of the entire system (watts)
$\bar{\nu}$ = average fission neutrons per fission event
Q = average recoverable energy (excludes neutrinos) per fission event (Joules/fission)
k_{eff} = eigenvalue of the system

There have been extensive discussions on the correct interpretation of variables in Eq. (2) and procedures for their evaluation suggested [11]. The ambiguity lies within the value of Q. It takes some effort to calculate this average value over an entire system having different actinides among the active cells. As burnup proceeds, the actinide species vary correspondingly. ORIGEN employs the following relation to calculate recoverable energy per fission for each actinide including the energy of non-fission capture and decay energy [9]:

$$Q(Z, A)\ (\mathrm{MeV/fission}) = 1.29927 \times 10^{-3}\left(Z^2 A^{0.5}\right) + 33.12, \tag{3}$$

where Z and A are the atomic number and atomic mass, respectively. Therefore, the average recoverable energy also changes with burnup. In addition, both k_{eff} and $\bar{\nu}$ are needed. As discussed in Ref. [11], scaling by k_{eff} for non-critical systems (mostly the case in burnup calculations) also carries uncertainties, since although fission rates scale well with k_{eff}, one-group fluxes may not.

A more rigorous and conceptually-transparent way is to obtain the flux multiplication factor based on an energy balance as follows:

$$\mathrm{FMF} = \frac{P}{\sum_{i=1}^{n}\sum_{j=}^{m_i} N_{ij}\left[\int \sigma_{ij,f}(E)\phi_i(E)dE\right]V_i Q_j} \tag{4}$$

where P = total power of the system
N_{ij} = the number density of actinide j in active cell i
$\sigma_{ij,f}(E)$ = fission cross section of actinide j in active cell i
$\phi_i(E)$ = spatial-average neutron spectrum in active cell i

V_i = volume of active cell i
Q_j = recoverable energy for actinide j
m_i = total number of actinides in active cell i

Equation (4) appears more complex than Eq. (2). However, all quantities involved are transparent and readily available during the computational process and evaluation of Eq. (4) takes a negligible fraction of CPU time in comparison to MCNP runs. Moreover, Eq. (4) together with Eq. (3) is fully compatible with the ORIGEN2 depletion scheme. Thus, Eq. (4) was implemented in MCODE. The flux multiplication factor is also calculated using Eq. (2) and reported in the detailed output file. Equation (2) is implemented in MONTEBURNS. MOCUP reads the normalization factor from a separate input file and its supply is left to the user's responsibility. Fundamentally there is no conceptual difference between these two equations; both give the instantaneous flux multiplication factor.

2.3 ORIGEN DEPLETIONS

ORIGEN is the depletion module incorporating MCNP-calculated one-group cross sections and flux values for each active cell. There are two modes of depletion, either constant power (IRP in ORIGEN) or constant flux (IRF in ORIGEN), which implies that either power or flux will be constant for each active cell within the timestep. In reality the overall power of the system is usually maintained at a certain level under steady state operations. The constant-power depletion mode can ensure a certain energy production for a given timestep. However, the constant-flux depletion mode can not guarantee the desired energy production because the beginning-of-timestep flux can only ensure the beginning-of-timestep power level. In order to facilitate user self-checking and MCODE functionalities, a special procedure is needed for the constant-flux depletion mode.

Under constant flux depletion, the average flux through the timestep is needed. This is accomplished by applying a so-called internal burnup corrector in ORIGEN, as proposed in [11], according to the following procedure:

1. Extract one-group cross sections and flux values from MCNP output
2. Calculate the flux multiplication factor and obtain beginning-of-timestep flux values
3. Execute a trial ORIGEN run with constant beginning-of-timestep flux values
4. Compute the ratio of energy production between rated power and the trial ORIGEN run (average to beginning-of-timestep ratio)
5. Use the average to beginning-of-timestep ratio to correct beginning-of-timestep flux values
6. Re-run ORIGEN with adjusted constant timestep-average flux and obtain final results.

This internal burnup corrector technique in ORIGEN ensures validity of constant-flux-mode depletion. The expense to be paid is running ORIGEN twice per timestep, which is unimportant since the fraction of CPU time of ORIGEN runs is negligible compared to MCNP running time.

Under constant power depletion, the power is guaranteed as the rated power. Power fractions for each active cell are calculated as follows:

$$f_i = \frac{\sum_{j=1}^{m_i} N_{ij} \left[\int \sigma_{ij,f}(E) \phi_i(E) dE \right] V_i Q_j}{\sum_{k=1}^{n} \sum_{j=1}^{m_k} N_{kj} \left[\int \sigma_{kj,f}(E) \phi_k(E) dE \right] V_k Q_j} \tag{5}$$

where symbols have the same meaning as in Eq. (4). Then, the power of each active cell is determined by multiplying the given total power with the fraction factor.

2.4 COUPLING BETWEEN MCNP AND ORIGEN

The coupling between MCNP and ORIGEN needs to be given special attention. Because the cross sections, flux values and power fractions in active cells undergo continuous changes with time throughout reactor operation, beginning-of-timestep values are not fully representative of the entire timestep, unless the timestep is exceedingly small. Better estimates of timestep-average values are needed.

In our formulation, denote the timestep as $[t_{n-1}, t_n]$. The material vectors $\mathbf{X}_i$, $i = 1, 2, \cdots, n$ are known at t_{n-1}. The question is then how to solve Eq. (1) to obtain end-of-timestep values. One thing to note is that Eq. (1) can also be written in vector form:

$$\frac{d\mathbf{X}_i(t)}{dt} = \mathbf{A}_i(t)\mathbf{X}_i(t), \qquad i = 1, 2, \cdots, n \tag{6}$$

where the matrix **A** is called the transition matrix.

In MOCUP, beginning-of-timestep cross sections and flux values in active cells are assumed constant over the entire timestep. Then, the analytic solution at the end of the timestep is

$$\mathbf{X}_i(t_n) = \exp(\mathbf{A}_i(t_{n-1})\Delta t)\mathbf{X}_i(t_{n-1}) \tag{7}$$

In MONTEBURNS, the so-called middle timestep approach is deployed, i.e., the middle-of-timestep values are extracted to build the transition matrices to represent the entire timestep, namely

$$\mathbf{X}_i(t_n) = \exp\left(\mathbf{A}_i\left(\frac{t_{n-1} + t_n}{2} \right) \Delta t \right) \mathbf{X}_i(t_{n-1}) \tag{8}$$

In MCODE, a standard predictor-corrector approach is implemented [12]. The burnup depletion is calculated twice, first using the spectra corresponding to the isotope vector at the start of the step and then, after a new spectrum calculation, using the spectra at the end of step. Average number densities from these two calculations are taken as the end-of-timestep material compositions.

$$\begin{aligned} \mathbf{X}_i^{\mathrm{P}}(t_n) &= \exp(\mathbf{A}_i(t_{n-1})\Delta t)\mathbf{X}_i(t_{n-1}) \\ \mathbf{X}_i^{\mathrm{C}}(t_n) &= \exp(\mathbf{A}_i^{\mathrm{P}}(t_n)\Delta t)\mathbf{X}_i(t_{n-1}) \\ \mathbf{X}_i(t_n) &= \frac{\mathbf{X}_i^{\mathrm{P}}(t_n) + \mathbf{X}_i^{\mathrm{C}}(t_n)}{2} \end{aligned} \tag{9}$$

It is obvious that the simple and computationally straight-forward approach adopted in MOCUP is the least accurate approximation of the three. MONTEBURNS is better in terms of computer running time savings than MCODE. However, the standard predictor-corrector algorithm is more accurate and is the preferred algorithm for burnup calculations for all licensing-level reactor physics codes, such as CASMO-4 [13] and HELIOS. Conceptually it is better than the middle-timestep approach in MONTEBURNS since it better accounts for the non-linear behavior of transition matrices. Even with large timesteps and bad statistical precision, MCODE still obtains fairly good eigenvalue histories. One disadvantage of the middle-timestep approach is the effect on iteration procedures because eigenvalues will be calculated at the middle of the timestep, not at the end of the timestep. If eigenvalues at the end of timestep are needed, additional MCNP runs are required. With advances in computation power, the impact of doubling the running time of MCNP will be less significant for burnup calculations.

Comparisons of MCODE with MOCUP and MONTEBURNS are summarized in Table 1.

Table 1. MCODE comparisons with MOCUP and MONTEBURNS.

	MCODE	MOCUP	MONTEBURNS
Developer	MIT	INEEL	LANL
Year	2001	1995	1999
Language	ANSI C	ANSI C	FORTRAN + PERL
Portability	excellent	good	good
User involvement	small	extensive	small
Running Flexibility	excellent	excellent	good
Normalization	power or flux	flux	flux
Coupling manner	Standard predictor-corrector algorithm	Beginning-of-timestep representation	Middle of timestep representation

3. HIGH BURNUP UO_2 LATTICE BENCHMARK

3.1 PIN CELL MODEL

A single pin cell model (Figure 2) of a standard Westinghouse 17×17 PWR assembly has been employed to benchmark MCODE. Boundaries of the unit cell are set to be reflecting. This model represents the cross section (two-D) of the fuel pin while ignoring axial dependence (in MCNP the pin cell is 4 cm in height with top and bottom reflecting boundaries). In order to use the ENDF/B-VI MCNP libraries provided with the code, isothermal cold conditions (room temperature, 300K) are used. The fuel is uranium dioxide with 9.75 w/o U-235 enrichment which results in high burnup (~100MWd/kg). It is, therefore, a challenge to MCODE since large numbers of actinides and fission products are needed. Since this is well above the current burnup licensing limit of 60 MWd/kg, it is also a challenge to CASMO-4 and HELIOS (two available deterministic codes). Note that all the codes treat the entire fuel region as one lumped block. Actual calculations show that refinement of fuel (dividing the fuel pellet into several concentric regions) gives almost the same results. Detailed pin cell model parameters are shown in Table 2 and the initial compositions are shown in Table 3.

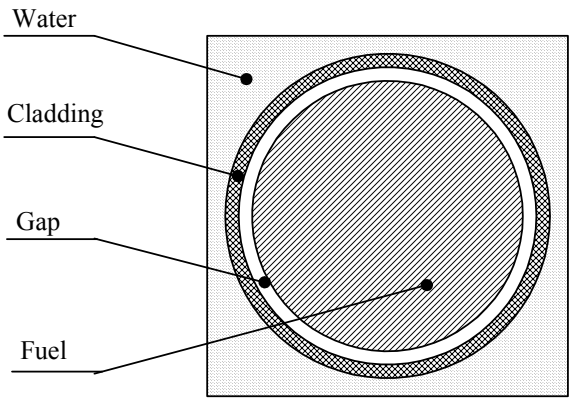

Figure 2. Pin cell model (not to scale).

Table 2. Pin cell model parameters (cold conditions at 300 K).

Parameters	Values
Fuel pellet radius (cm)	0.4096
Cladding inner radius (cm)	0.4178
Cladding outer radius (cm)	0.4750
Pin pitch (cm)	1.26
Fuel density (g/cm^3)	10.3
Cladding density (g/cm^3)	6.550
Coolant density (g/cm^3)	0.997
Power density (kW/liter core)	104.5
Specific power (W/gU)	34.6679

Table 3. Initial compositions (cold conditions at 300 K).

	Nuclide	Weight percent (w/o)	Number density (1/cm^3)
Fuel (9.75 w/o UO_2)	U-234	0.0688	1.82239E+19
	U-235	8.5946	2.26826E+21
	U-238	79.4866	2.07128E+22
	O-16	11.8500	4.59686E+22
Cladding (Zircaloy-4)	O	0.125	3.08281E+20
	Cr	0.10	7.58663E+19
	Fe	0.21	1.48338E+20
	Zr	98.115	4.24275E+22
	Sn	1.45	4.81835E+20
Coolant (H_2O)	H-1	11.19	6.66295E+22
	O-16	88.81	3.33339E+22

3.2 CODE DESCRIPTIONS

Results of MCODE were benchmarked against CASMO-4 [13] and HELIOS. Those two codes are licensing-level, industry standard burnup calculation tools, which solve the transport equation based on deterministic methods. One thing to note is that CASMO-4 uses neutron cross section libraries

processed from JEF-2.2 and ENDF/B-6; while MCODE is entirely based on ENDF/B-6 library data. However, we still use CASMO-4 as the reference and use HELIOS results to double check its validity. The main features of each code are summarized in Table 4:

Table 4. Summary of benchmarking codes [11].

	MCODE	CASMO-4	HELIOS
Cross section libraries	ENDF/B-6	ENDF/B-6, JEF2.2	ENDF
Code developer	MIT	Studsvik	Scandpower
Transport treatment	Monte Carlo	KRAM characteristics	CPM+CCPM
Resonance treatment	Monte Carlo	collision probability	subgroup method
Number of energy groups	continuous	70	45
Burnup algorithm	predictor-corrector	predictor-corrector	predictor-corrector
Leakage	No	No	No
Actinide representation	39	Th231 thru Cf252	Th230 thru Cm246
Fission products	100	~200	115

3.3 RESULTS AND ANALYSIS

Forty-nine burnup steps are chosen between 0 and 100 MWd/kg for the benchmarking calculations. The running options for MCODE are power normalization with burnup predictor-corrector algorithm on. There are 39 actinides (ACT) and 100 fission products (FP) considered in the burnup calculations, which accounts for ≥ 99.95% total mass and neutron absorptions. Mass conservation is preserved. Each MCNP run takes about 1 hour with 225,000 neutron histories and the entire run takes about 4 days with MCODE using a DEC alpha workstation. Figure 3 shows the comparison of eigenvalue history among MCODE, CASMO4, and HELIOS, and Figure 4 shows the difference from CASMO-4.

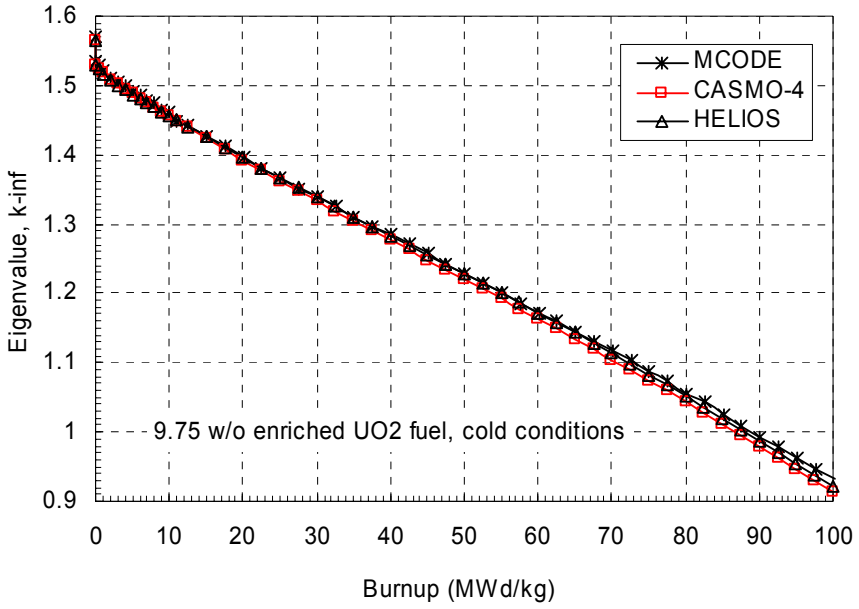

Figure 3. Eigenvalue comparison between MCODE, CASMO-4, and HELIOS.

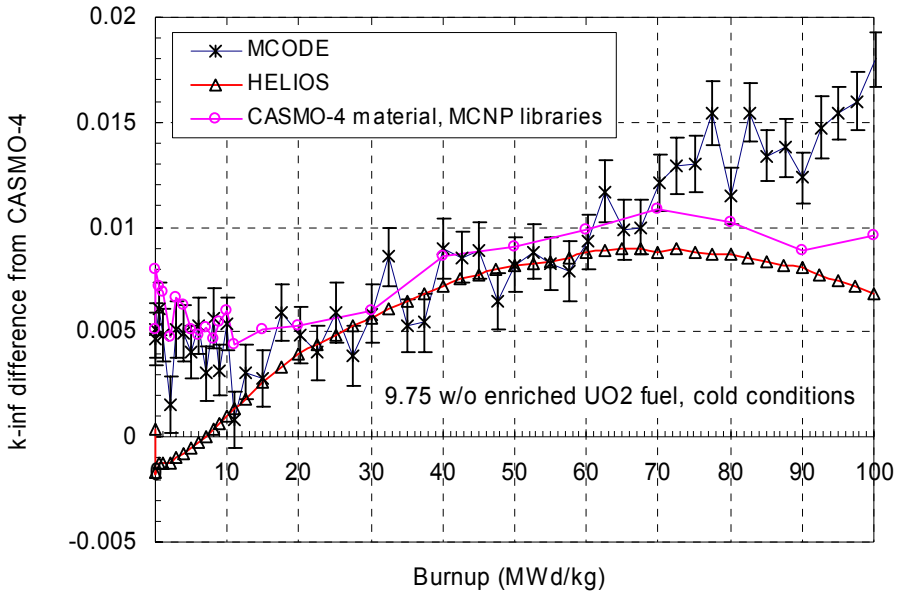

Figure 4. Eigenvalue difference from CASMO-4 as a function of burnup.

It can be seen from Figure 4 that before 60 MWd/kg there is a nearly a constant Δk between MCODE and CASMO-4. Then it grows almost in a linear way. HELIOS agrees with CASMO-4 better than MCODE. At 100 MWd/kg burnup, the eigenvalue difference is about 0.015. This is comparable to previous benchmark efforts [11] where the eigenvalue difference reaches 0.01 at 60MWd/kg. Circled points indicate MCNP criticality calculations using the CASMO-4 output material vectors and MCNP libraries. This isolates the static library difference and shows that the constant Δk before 80MWd/kg is mainly the library difference. Even at 100 MWd/kg, the static library difference still accounts for about two thirds of the eigenvalue discrepancy between MCODE and CASMO-4. In addition, the dynamic library difference should also be taken into consideration, i.e., the burnup effect from library differences. From the authors' experience, it appears that there are more fertile isotopes converted to fissile in MCODE than in CASMO-4 which phenomenologically explains the eventual linear increase in eigenvalue difference. Several other causes might also contribute, such as statistical error propagation, or empirical treatments in CASMO-4 or HELIOS. From an engineering point of view, MCODE is sufficiently accurate and gives consistent results.

In addition to eigenvalue comparison, an isotope composition comparison at 100 MWd/kg is also presented along with uncertainties for uranium fuel from [7]. Note that these uncertainties are given as the spread of isotope concentrations from dozens of calculations. The referenced numbers are results for 44.34 MWd/kg burnup UO_2 fuel while our comparison is at a more challenging 100MWd/kg.

Table 5 confirms that there are overall more fissile species present for MCODE. Most of the material compositions agree with CASMO-4 within typical uncertainties. Taking into consideration the high burnup the differences are mostly acceptable. Also, it is clear from Table 5 that the fissile excess can be attributed to higher consumption of U-238, which results in more Pu-239 and less U-235 consumption.

From the code-vs-code benchmarking of the high burnup UO_2 lattice under cold conditions, it is

concluded that MCODE is suitable and ready to be used in burnup calculations. Even under high burnup cases, the eigenvalue comparisons are still within ~0.02 of CASMO-4, and even closer to HELIOS. The material composition predictions are also acceptable compared to the comprehensive uranium benchmark reported by OECD.

Table 5. Fractional difference from CASMO-4 in nuclide concentration at 100 MWd/kg.

Isotopes	CASMO-4 (#/cm^3)	HELIOS	MCODE	Max typical uncertainties [7]
Mo-95	1.22281E+20	NA	–0.17%	1.85%
Tc-99	1.16862E+20	NA	4.54%	4.21%
Ru-101	1.19274E+20	NA	–0.30%	1.76%
Rh-103	4.60151E+19	NA	3.30%	5.40%
Ag-109	6.99101E+18	NA	14.62%	10.21%
Cs-133	1.14516E+20	NA	8.15%	5.60%
Cs-135	6.98202E+19	NA	0.35%	3.63%
Nd-143	7.42463E+19	NA	0.34%	4.51%
Nd-145	7.10908E+19	NA	–0.08%	1.46%
Sm-147	9.57151E+18	NA	14.09%	9.12%
Sm-149	1.24554E+17	NA	–5.83%	15.61%
Sm-150	2.67571E+19	NA	8.08%	8.50%
Sm-151	7.68167E+17	NA	–10.27%	22.31%
Sm-152	9.39450E+18	NA	–16.19%	9.68%
Eu-153	1.18378E+19	NA	–11.36%	8.52%
U-234	6.71252E+18	0.86%	1.20%	8.99%
U-235	2.59522E+20	–1.24%	2.10%	8.12%
U-238	1.96718E+22	–0.11%	–0.17%	2.60%
Np-237	3.42341E+19	0.98%	–8.90%	9.42%
Pu-238	1.96654E+19	–0.08%	–8.26%	13.86%
Pu-239	1.47667E+20	2.05%	5.61%	7.12%
Pu-240	6.31059E+19	6.49%	8.77%	5.27%
Pu-241	4.28013E+19	1.21%	5.13%	6.86%
Pu-242	2.62275E+19	–3.92%	–3.05%	8.39%
Am-241	2.35052E+18	–4.40%	9.96%	5.29%
Am-243	6.23202E+18	19.86%	23.22%	10.40%
Total actinides	2.02803E+22	–0.08%	–0.07%	NA
Total fissile	4.92807E+20	0.37%	2.96%	NA
Total fertile	1.97875E+22	–0.09%	–0.15%	NA

4. AXIALLY HETEROGENEOUS UO_2/ ThO_2 PIN CELL

4.1 INTRODUCTION

One of the great advantages of Monte Carlo codes over deterministic codes is the capability to deal with complex geometries and heterogeneous configurations. In this part, use of MCODE is demonstrated on an innovative heterogeneous thorium-uranium fuel design [8].

In recent years thorium has attracted considerable interest, primarily because of the potential proliferation-resistance of the Th232/U233 fuel cycle. An innovative axially heterogeneous ThO_2/UO_2 fuel was proposed and studied by Xianfeng Zhao at MIT [8] to enhance neutronic sustainability (burnup). The basic idea is to separate thorium from uranium by axially stacking zones of each type of pellet. The MCNP model for Ax4 is shown in Figure 5:

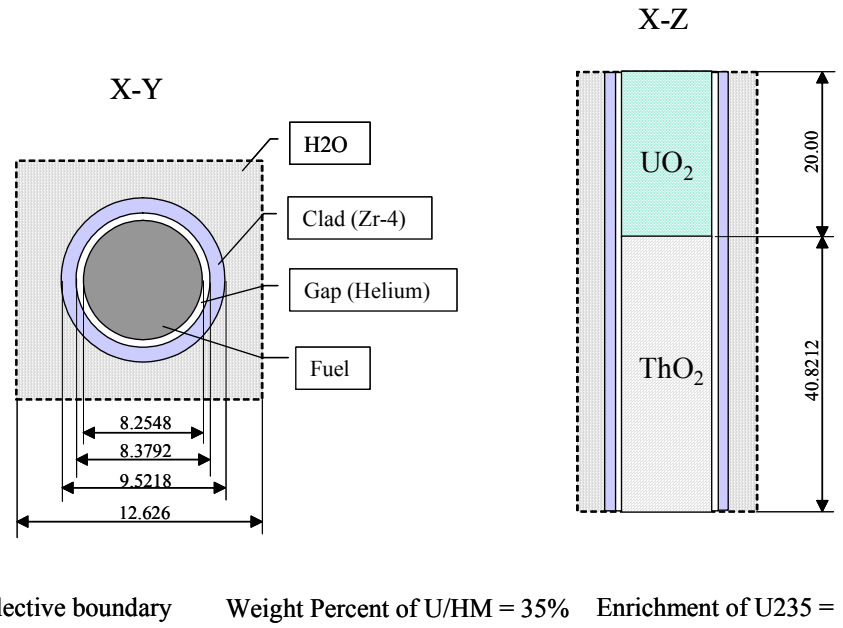

Figure 5. Illustration of Ax4 case (dimensions in mm).

From the code development point of view, this is a good test (large local spectrum difference) for MCODE. Although the model is still a pin cell model, there are abrupt material-change interfaces in the fuel which makes Ax4 a genuine 3-dimensional problem. There is a steep rise in power of the ThO2 segment as U-233 builds up from Th-232. There is also a strong coupling/interaction between UO_2 and ThO_2 segments. None of the available deterministic transport codes can handle this case.

4.2 RESULTS AND DISCUSSIONS

For simplicity, the Ax4 case is modeled with two active cells in MCODE, one is the UO_2 segment and the other is the ThO_2 segment. Several calculations using different options in MCODE have been done to show the value of the predictor-corrector algorithm and to provide some guidance for use of MCODE options.

Twenty-seven timesteps are chosen between 0 and 95 MWd/kg. In principle, the results should not depend on the method of normalization. Thus, both power and flux normalizations are compared. In addition, the predictor-corrector option is also applied. Altogether, four cases were initiated using the same burnup scheme. There are 225,000 neutron histories for each MCNP run which takes about 30 minutes. A limited number of fission products (41) and actinides (17) are chosen to reduce MCNP

running time. The entire run for each case takes about 1 day using a Pentium-IV 1.8 GHz CPU. One additional coarse MCODE run with 2250 neutron histories (hence higher statistical error) for each MCNP run, and larger timesteps were also tried. Table 6 summarizes these runs:

Table 6. MCODE runs with various options for Ax4.

	Neutron histories in each MCNP run	Normalization option	Predictor-correction option	Total running time (hours)
Case 1	225,000	Power	OFF	9
Case 2	225,000	Flux	OFF	9.5
Case 3	225,000	Power	ON	18
Case 4	225,000	Flux	ON	19
Case 5	2250	Flux	ON	1

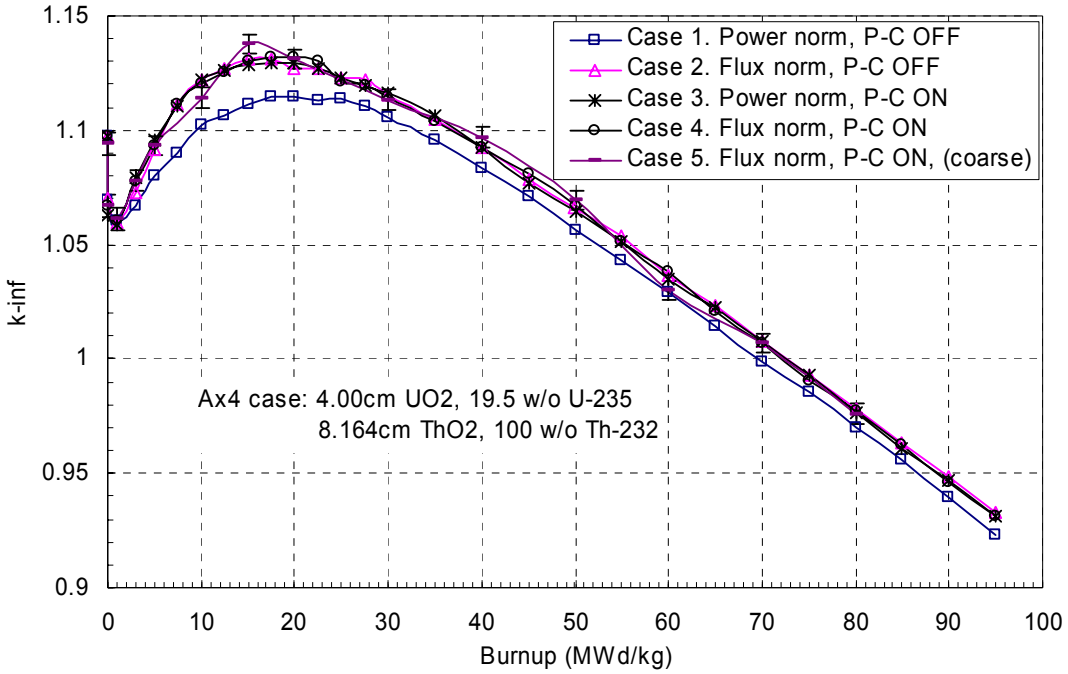

Figure 6. Eigenvalue histories for different run options.

In Figure 6, the only points of case 5 are plotted together with their standard deviations. Standard deviations of other cases are about one fifth those of case 5. Several things of interest can be seen from this figure. First, case 1 disagrees with all other cases while cases 2 to 5 are in good agreement. Because no licensing-level deterministic codes can deal with this axially heterogeneous case, other approaches must be employed to identify the sources of the differences. The constant power and no-predictor-corrector case 1 implies that the ThO_2 and UO_2 cells deplete at the beginning-of-timestep power throughout the entire time step. This is not a good assumption here, however. As can be seen from Figure 7, the power in ThO_2 increases from ~0 to a significant level with burnup as U-233 builds up.

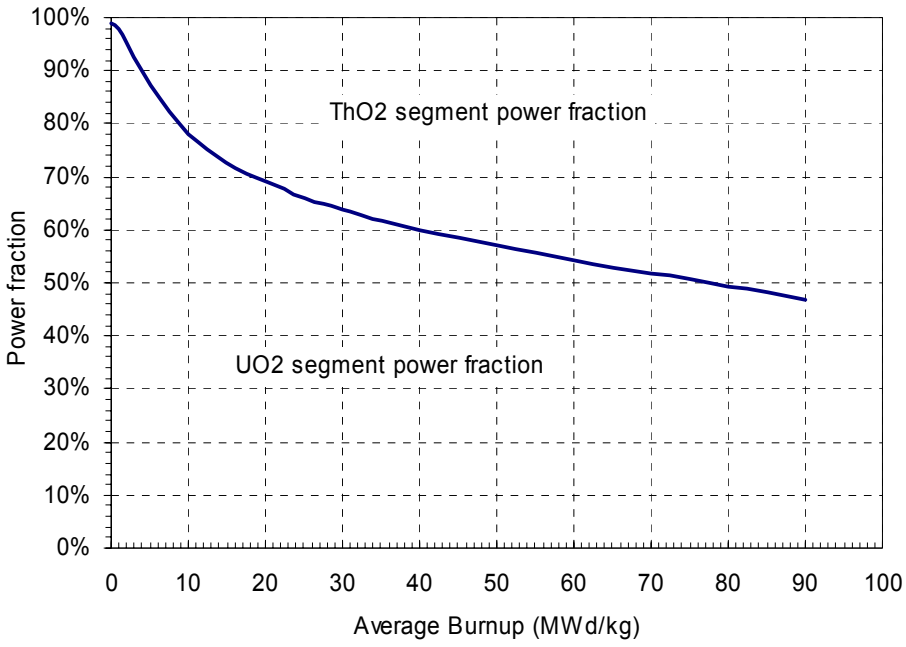

Figure 7. Power sharing between UO_2 and ThO_2 as a function of burnup.

In particular before 15 MWd/kg, use of the beginning-of-timestep power significantly lowers the thorium power sharing, which results in an over-burn of UO_2 fuel and less U-233 generated in thorium. The eigenvalue grows more slowly than in the other cases. If one turns on the predictor-corrector (case 3), results show a correct trend in behavior. The predictor-corrector therefore proves its importance here. Even with high MCNP statistical errors and large timesteps as in case 5, the predictor-corrector still follows closely the consensus best-estimate burnup curve, although there are notable oscillations with burnup due to the bad statistics. This study confirms that the standard burnup predictor-corrector algorithm is needed for reactor design calculations. Case 1 underestimates the burnup by about 3 MWd/kg in terms of B_1(k = 1.03 to account for leakage).

It is surprising to see that case 2 (flux normalization, no predictor-corrector) agrees with the "best" burnup curve. Figure 8 does show that the flux ratio between UO_2 and ThO_2 segments changes slowly with burnup. Thus, the beginning-of-timestep flux ratio is representative of the entire timestep average flux ratio and the burnup predictor-corrector can be turned off.

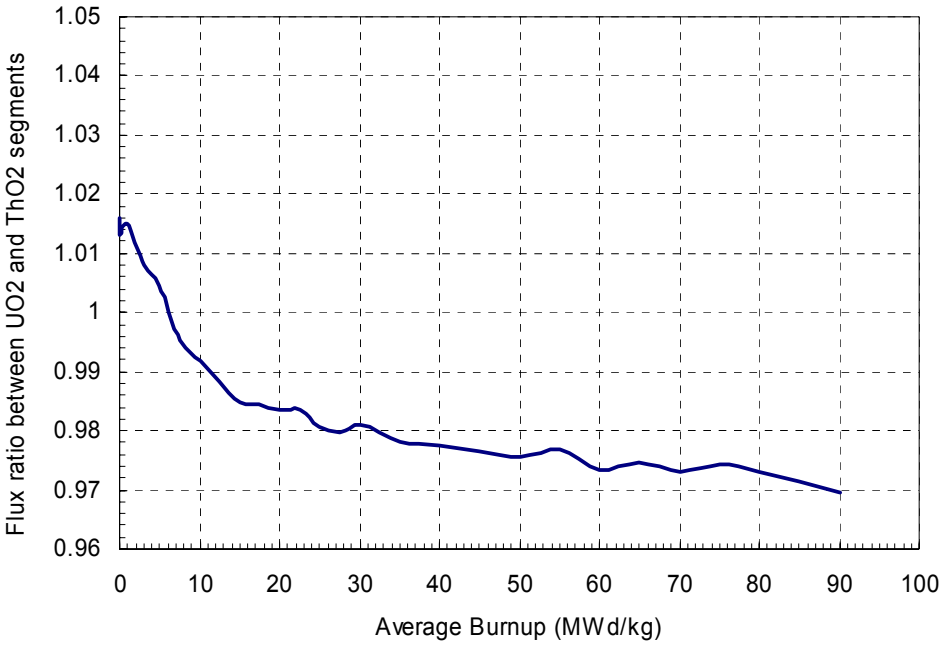

Figure 8. Neutron flux ratio between UO_2 and ThO_2 segments.

4.3 SUMMARY

MCODE has been demonstrated to be able to solve the axially heterogeneous UO_2/ThO_2 fuel problem, and some general guidelines for choosing normalization and predictor-corrector options have been established:

- Whenever CPU time permits, the burnup predictor-corrector algorithm should be turned ON, and results should be independent of normalization options. In that situation, the power normalization option is recommended in preference to the flux normalization option.
- If one is limited by computer time and cannot use the burnup predictor-corrector, flux normalization is then recommended. The output file should be double checked to verify that there are no significant relative changes among flux values in each active cell.

5. CONCLUSIONS AND RECOMMENDATIONS

MCODE — a linkage code between MCNP and ORIGEN — has been developed at MIT. Compared to other linkage codes, it has better usability and improved functionalities. The methodology is described and some particular aspects are emphasized. The approach to coupling MCNP and ORIGEN makes the code unique. Benchmark calculations of a high burnup UO_2 PWR lattice under cold conditions show fairly good agreement with licensing-level codes. The material composition differences mostly lie within the range of previous benchmark studies, even at a higher burnup

(100MWd/kg). Intrinsic differences are also revealed between cross section libraries in MCODE and libraries in CASMO-4. The second example applying MCODE to axially heterogeneous thorium/uranium fuel is also interesting. Based on several ways of running MCODE, general guidelines for running MCODE are discussed. If time permits in a given application it is recommended that the burnup predictor-corrector algorithm should be turned on; and power normalization rather than flux normalization is recommended. One should also be aware of the powerful MCNP modeling capability although only simple geometries are adopted in the two cases for illustration/verification purposes. For example, MCODE has been applied to fast actinide burner cores with sophisticated lattice geometries.

Future work is needed to 1) develop temperature-dependent libraries to simplify the nuclide selection process in MCODE; 2) develop a perturbation method that can greatly reduce second MCNP step running time in the corrector. Also the propagation of statistical errors should be studied to establish a rough estimate of the deviation of material number densities at individual time steps compared to desired precision. The ORIGEN data, such as fission yields and one-group cross section libraries, should be updated to improve MCODE precision.

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