Visualization of Coupled Spectral and Burnup Calculations: an Intuition-building Tool

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Abstract

In this paper, we present a fast, user-friendly computational tool for the calculation and visualization of coupled neutron spectra and fuel burnup calculations. This tool, V:BUDS (visualize: burnup, depletion, spectrum), was designed to derive scenario-dependent material balances for fuel cycle systems studies. While V:BUDS does not replace more high-fidelity models, its simple interface, short computation time, and graphical output format make it a useful tool for classroom demonstration or student experimentation with a wide range of reactor phenomena. V:BUDS is a C-based code bundled with custom cross section libraries and driven by a graphical MATLABTM front end. It operates at the unit cell level and couples a detailed multigroup treatment of energy dependence with a simplified collision probability model of spatial dependence. This approach gives strong fidelity to benchmarked standards for LWRs and responds correctly to perturbations in relevant parameters such as geometry and composition.

1. Introduction

Familiarization with the setup and execution of coupled transport/burnup calculations, using for instance the MCNP/MOCUP, SCALE or WIMS code packages, is an essential component of many reactor physics curricula. Although imparting a crucial, marketable skill to learners, exclusive reliance upon these necessarily slow, complex and outcome-oriented licensing-quality packages in teaching computational reactor physics could short-change students in one important respect. This may broadly be referred to as intuition building: how do the burnup-dependent spectrum, multiplication factor, reactivity coefficients and isotopic composition respond to changes in geometry, initial number densities, temperature and residence time?

A new tool, V:BUDS (visualize: burnup, depletion, spectrum) has been developed to fill this gap. The V:BUDS computational engine, originally developed to provide material balances for fuel cycle system studies, uses a few spatial region collision probability formulation to treat the spatial dependence of the flux. This is coupled with a multigroup treatment of energy dependence incorporating a hyperfine (740 group) or traditional (110 group) mesh. V:BUDS is bundled with custom cross section libraries, evaluated from the ENDF-B/VI data using NJOY99 and covering the temperature range 300 – 1500 K. The libraries include fuel matrix, cladding,

moderator, coolant and structural materials typical to thermal and fast spectrum facilities. V:BUDS is suitable for dynamic, in-class use as a hands-on tool: it calculates spectra in under one second on a typical machine and completes a depletion calculation incorporating burnupdependent spectra in under ten seconds.

The V:BUDS visualization system uses MATLAB to invoke C routines where most of the computations are performed. V:BUDS produces movies – with each frame representing a time, burnup or fluence step – of energy-dependent spectra as well as groupwise interaction rates and self-shielded cross sections for user-specified nuclides. Dynamic plots of reactivity coefficients, buildup and one-group cross section by isotope, multiplication factor, and all coefficients of the six-factor formula are also available. Some of the reactor physical considerations that may be demonstrated to students include the effect of fuel and nonfuel temperature on the spectrum and isotopic buildup, spectral behavior as lattice geometry and the fuel volume ratio are varied, the effect and propagation of changes in initial component number densities, the reactivity worth of individual component materials and nuclides and their evolution with burnup, energy and concentration-dependent self shielding, trends in reactivity coefficients, and the impact of uncertainties in cross section data on system performance.

In this paper we demonstrate the use of V:BUDS to conduct these intuition-building exercises. An overview of the V:BUDS methodology and input/output framework is provided in Section 2. Section 3 presents a list of learning objectives for a classroom demonstration and summarizes the sample case to be analyzed. This case is a typical MOX cycle, drawn from Phase IV-B of the OECD/NEA Burnup Credit Criticality Benchmark. Through consideration of this basic cycle and application of a suite of perturbations, the intuition-building exercises listed above will be carried out and presented as classroom lessons in Section 4. It will be demonstrated that, since V:BUDS executes quickly and perturbations are easily applied, 'what if?' questions from students may be immediately answered with easy to interpret graphical output. We conclude in Section 5 with suggestions for use of V:BUDS as a learn-by-doing tool, with hands-on student experimentation serving to lay the intuitive groundwork for more effective use of design-suitable software packages.

2. Summary of V:BUDS Methodology

V:BUDS was initially developed to compute material balances for fuel cycle systems calculations. As such, it emphasizes generality of application and ease of use. The suitability of V:BUDS as a pedagogical tool follows from these features. In this section, we first summarize the physical basis of the V:BUDS methodology. More elaborate documentation is available in Ref. 1. The results of several benchmarking exercises are provided in Ref. 2. We also describe the V:BUDS input as well as its MATLAB-generated graphical output.

2.1. Reactor Physics

V:BUDS relies upon a multigroup formulation to treat energy dependence. The ENDF/B-IV data were processed using NJOY99³ to yield cross section libraries at 5 temperatures (300, 600, 900, 1200, 1500 K). Cross sections come bundled with V:BUDS for a wide range of potential constituents. These include 24 actinide isotopes, oxide, nitride, zirconia, and zirconium hydride fuel forms, common cladding and structural materials (*e.g.*, Zircaloy, HT-9), control absorbers

(boron, B₄C, Ag-In-Cd, Gd₂O₃) and a number of common moderators and coolants (light or heavy water, graphite, helium, CO₂, lead, bismuth and sodium). For a full listing of the coolant/moderator, structural and other non-fuel materials currently supported by V:BUDS, please refer to Ref. 1. Rather than adopt any of the currently existing energy meshes, V:BUDS uses energy grid in which all bins are of equal lethargy width. This mesh, which contains 10 (coarse representation) or 100 (fine) bins per neutron energy decade, was chosen because the set of isotopes whose resonances might determine the binning structure could vary widely between V:BUDS runs.

Spatial dependence is treated by a two-region collision probability formulation. The two regions, central and annular, may be chosen to conform to cylindrical, spherical or slab configurations. One of the regions can contain actinide isotopes.

2.2 Input Format and Output Visualization

V:BUDS is driven by a graphical user interface (GUI). This GUI allows the user to customize the geometry and composition of the cell to be studied, the temporal parameters governing a burnup calculation, and the outputs to be plotted. The figures below provide screenshots of the GUI windows; the inputs given in the figures describe one of the burnup credit benchmark cases, namely case number five of Ref. 7.

The GUI consists of two windows. In the first of these, shown in Figure 1, users may customize cell geometry and material composition. Supported geometries include cylindrical, cylindrical hexagonal-lattice, slab and spherical (for modeling pebble-type cells). V:BUDS supports the presence of actinides in either the central or the annular region of the cell, and its cross section libraries cover a number of fuel forms. For actinides, the composition is explicitly specified on an isotope-by-isotope basis. In the example shown in the figure, the actinide number densities drawn from Ref. 7 are used. These override the fuel density [g/cc] specified when the fuel form is selected. Sometimes, though, it is more convenient to specify only the mass fraction of each actinide in the fuel. In this case, V:BUDS derives the actinide number densities from the fuel density. V:BUDS uses a simple diffusion theory-based buckling model to estimate leakage; since the benchmark case studied here models an infinite lattice, the reactor dimensions are set to be very large.



Figure 1. The V:BUDS GUI, First Window

The dynamic and output options for the run are selected in the second GUI screen as shown in Figure 2. Here, users first select a *static* (fuel burnup not simulated; spectral calculation carried out for only the composition specified in Figure 1) or *time-dependent* (burnup and depletion calculation) run. V:BUDS computes and can plot the energy dependent flux spectrum, the neutron balance as expressed by neutron production and destruction rates for each species or by the terms of the six-factor formula, and selected reactivity coefficients. If the *static* option is chosen, these are presented as bar graphs or plots for the specified condition. If the *time-dependent* option is used, they are displayed as plots or movies incorporating the evolving composition of the fuel. Additionally, under this option users can choose to create plots of the relative or absolute prevalence of each of the explicitly tracked actinide isotopes. These outputs can also be saved as text files. We discuss the plots themselves as they are created in the course of the classroom demonstration: please refer to Section 4.

VBUDS: Run and Plot Options		×
Execution Options:	Dynamic Input / Output Options KY Plo	ots] Isotopes vs. BU / Time:
C Static (Calculate Given State Point)	Burnup Options:	Th-230
Time-Dependent (Burnup Calculation)	Discharge Burnup [MWd/kgIHM] 48	Pa-231
General Plotting Options	Cycle Uptime 420	U-233
For Neutron Production / Comsumption Plots and Graphs, Lump Species into 'Other' Spagnumber they Account for	Number of Cycles 3	□ U-234 □ U-235
Less than 5 %	Load Factor [%] 93.33	□ U-236 □ U-238
of the Total Production / Consumption. (Larger Number Makes Plots More Readable)	X-Axis for Dynamic Plots:	□ Np-237
Static Output Options	 Burnup [MWd/kglHM] 	 ✓ Pu-238 ✓ Pu-239
[Bar Graph] Neutron Production & Consumption by Species / Isotope	[XY Plot] Neutron Production & Consumption by Species / Isotope	✓ Pu-240 ✓ Pu-241
□ [Bar Graph] K effective and Six-Factor Formula Terms	[XY Plot] K effective and Six-Factor Formula Terms	✓ Pu-242 ✓ Am-241
[Bar Graph] Doppler, Void and	XY Plot] Doppler, Void and	Am-242m
	Femperature Headstrivity Coefficients Femperature Headstrivity Coefficients Femperature Headstrivity Coefficients Femperature Headstrivity Coefficients Femperature Headstrivity Coefficients	
/ Neutron Flux Profile	Hegion Neutron Flux Profile	✓ Cm-244
Neutron Flux Profile	Region Neutron Flux Profile	Cm-245
	60 Timestep for flux Y-A calculations [days]	wis for Isotopic Plots: Number Density [#/barn.cm]
Execute V:BUDS	5 Timestep for delpetion calculations [days] •	Mass Fraction [% of IHM]

Figure 2. The VBUDS GUI, Second Window

3. A Classroom Demonstration: Motivation

The demonstration presented here is intended for students who have developed a basic understanding of elementary concepts often covered in a first course on reactor engineering. Since space does not permit us to dwell in detail upon each concept that could be illustrated through use of V:BUDS, we instead list them without comment and urge the reader to hold them in mind as s/he peruses the output presented in the next section. The concepts include reactor criticality as measured by the multiplication factor, neutron energy spectra, spatial effects as described by diffusion or transport theory, buildup and decay as described by the Bateman Equations, and safety parameters such as temperature or void reactivity coefficients. We assume that students have been introduced to these topics, but that they are just beginning to apply them to realistic reactor systems in which results must be obtained with the aid of computational tools. Our objective will be to deepen student understanding of each of them.

Among the properties of the reactor, or more accurately the cell representation of the reactor, we might explore are the neutron energy spectrum, the group constants, and the effect of energy self shielding. Additionally, we address the multiplication factor through both the six-factor formula coefficients and the reactivity worth of individual components. Also we evaluate reactivity coefficients (moderator and fuel temperature, moderator void). Basic understanding of the interaction between the burnup evolution of the spectrum and that of the fuel isotopic composition as well as the overall neutron balance (as measured by isotope-specific production and destruction rates⁴ or by so-called "D factors"⁵) is also vital.

It is also useful to list those relatively basic concepts that V:BUDS cannot address in its present form. Since V:BUDS uses a simple, few-region collision probability model to treat the spatial flux distribution, a detailed spatial representation of the flux cannot be achieved. To facilitate this approach, V:BUDS assumes, rather than derives, the flux distribution within each geometric region, so that spatial self shielding is not fully treated. Additionally, as for any cell model, the effect of heterogeneity (such as might be illustrated by nodalization or explicit modeling of multi-cell or assembly-scale systems) is not captured. Finally, although the V:BUDS computational engine derives adjoint fluxes and importance functions, these are not yet used in evaluating results such as reactivity coefficients, nor are they displayed in the graphical output.

3.1 Description of the Case

It is useful to summarize the example case being implemented for the classroom demonstration. This is a reproduction of the calculations performed in the OECD/NEA Burnup Credit Criticality Benchmark, Phases IV-A⁶ and IV-B⁷. The benchmark, an international effort involving numerous participants using a wide range of code packages and nuclear data libraries, entails calculation of the burnup-dependent multiplication factor and isotopic composition of a MOX pin cell. We will follow Cases 1 and 10 of Ref. 6 for the multiplication factor and reactivity coefficient computation and Case 5 of Ref. 7 for the burnup calculation.

Figure 3 shows the configuration of the equivalent unit cell used in Phase IV-B; the cell used in the criticality calculations of Phase IV-A varies slightly. The calculations are carried out assuming an infinite square lattice of these cells.



Figure 3. Unit Cell Used in Benchmark and Demonstration

The benchmark considers several initial plutonium vectors and burnup histories. We will choose vector 'A,' which corresponds to plutonium recovered from 5 year cooled medium-burnup UOX, as the starting point for our demonstration. The unperturbed initial fuel number densities are

shown in Table 1. Ref. 6 provides compositions for this fuel after irradiation to 20, 40 and 60 MWd/kg; these are also given in Table 1. The infinite medium multiplication factor and selected reactivity coefficients, with fission products absent and present, are evaluated for each of these four compositions. The calculations are carried out at room temperature.

Isotope	Number Density [atoms/barn-cm] at B =			
	0 MWd/kg	20 MWd/kg	40 MWd/kg	60 MWd/kg
U-234	2.800e-7	6.360e-7	7.772e-7	9.167e-7
U-235	5.857e-5	4.222e-5	2.902e-5	1.918e-5
U-236		3.725e-6	6.175e-6	7.536e-6
U-238	2.307e-2	2.273e-2	2.237e-2	2.199e-2
Pu-238	2.470e-5	2.279e-5	2.550e-5	2.951e-5
Pu-239	8.062e-4	5.918e-4	4.503e-4	3.633e-4
Pu-240	3.130e-4	3.145e-4	2.907e-4	2.561e-4
Pu-241	1.653e-4	1.825e-4	1.813e-4	1.653e-4
Pu-242	5.398e-5	7.059e-5	9.173e-5	1.121e-4
Np-237		1.613e-6	3.075e-6	4.200e-6
Am-241		1.843e-5	2.230e-5	2.157e-5
Am-243		1.353e-5	2.402e-5	3.257e-5

Table 1. Number Densities of Actinides in MOX Fuel

For the burnup calculations of Phase IV-B (Ref. 7), a very similar initial plutonium vector is used. The MOX is irradiated at constant power density to a discharge burnup of 48 MWd/kg in three cycles. Each cycle is 420 days in duration, followed by a 30 day downtime. The fuel temperature is taken to be 900 K, while the moderator is held at 575 K. The central result of this exercise is actinide number densities at the conclusion of each cycle.

4. A Classroom Demonstration: Execution

In this section we present a classroom narrative of the benchmark calculation, accompanied by screenshots from V:BUDS. All the figures shown here are produced by V:BUDS as MATLAB figures. We also discuss perturbations to the calculation that might arise from student questions or demonstrate additional concepts. The narration begins with an illustration of the k_{inf} for the cell for the initial and final actinide compositions. We illustrate two mechanisms for understanding the overall neutron balance.

The first of these is the contribution of each component to the neutron production and consumption rates. This is shown in Figure 4. In this and the subsequent two figures, the illustration at left shows the result for the fresh plutonium vector, while that at right reflects the actinide composition after 60 MWd/kg of burnup. V:BUDS normalizes the bar graphs such that the total neutron consumption rate in the unit cell equals unity. Additionally, there is a user-specifiable option, visible in Figure 2, to limit the display to those species contributing more than a given percentage to the total. In Figure 4, this percentage was set to 5%; hence, a number of actinide and other species not crossing this threshold are lumped into the 'Other' category.



Figure 4. Relative Neutron Production and Consumption Rates for Fresh (Left) and 60 MWd/kg (Right) Fuel Compositions

Figure 4, in this case, shows that fissile Pu-239 and 241 effectively dominate production. The depletion of Pu-239 is evident. Students might be interested to see that a few percent of neutrons are consistently produced through fast fission in U-238. Since this run is carried out at a temperature of 300 K with unit density water, it reflects a softer spectrum with less Doppler broadening than might be evident under reactor operating conditions. The temperature and density changes that would model such conditions are carried out for the burnup calculations and presented below.

This figure, when considered in conjunction with number densities, can help students understand one group cross sections. Students can easily be familiarized with pointwise infinitely dilute cross sections, but the convolution of these cross sections with flux spectra – leading to the one-group quantities – may be obscure at first. V:BUDS reaction rate illustrations for a variety of thermal and fast spectrum systems can help students understand how widely these one-group constants may vary for a given nuclide.

Reactor criticality as measured by the behavior of the multiplication factor can also be understood through the coefficients of the six-factor formula. This is given by

$$k_{eff} = \eta f p \varepsilon L_f L_t, \quad (1)$$

where k_{eff} is the multiplication factor. The other terms are defined as follows:

 L_{f} , the fast nonleakage probability, the probability that a fast neutron will not leak,

 L_t , the thermal nonleakage probability, the probability that a thermal neutron will not leak,

 ε , the fast fission factor, the number of neutrons produced through fission at all energies divided by the number produced by thermal fission,

p, the resonance escape probability, the fraction of nonleaking fast neutrons that succeed in slowing down to thermal energies,

f, the thermal utilization, the fraction of absorbed thermal neutrons that are absorbed in the fuel (defined as all actinides),

 η , the reproduction factor, the number of fission neutrons produced per thermal neutron absorbed in the fuel.

It may be beneficial to familiarize students with typical values of these quantities for an LWR through a V:BUDS run or from a text such as Ref. 8. Intuitive understanding can then be built through perturbations departing from this reference case. The discussion below will be developed assuming students already know what to expect for a 'generic' UOX-fuelled lattice.

Figure 5 shows the V:BUDS plots for the fresh and 60 MWd/kg fuel. It should be noted that the V:BUDS k_{eff} values agree with those published in the benchmark⁶ to better than 1%. V:BUDS sets the thermal/fast cutoff at 1 eV. This method of thinking about k_{eff} is seen to place a premium on understanding the energy distribution of neutrons, whereas the per-isotope neutron production and destruction discussed previously focuses on the characteristics of the individual species. One caveat: this approach to understanding k_{eff} has less value when the neutron spectrum is fast. Since so few neutrons are thermalized, ε will be orders of magnitude larger than all the other terms.



Figure 5. K_{eff} and 6-Factor Formula Terms for Fresh (Left) and 60 MWd/kg (Right) Fuel Compositions

The nonleakage probabilities are both unity in this case since V:BUDS simulated the infinite lattice used in the benchmark. The decrease in k_{eff} for the 60 MWd/kg fuel can be seen, though additional runs can show students that this drop is less dramatic than would be the case for UOX fuel. The fast fission factor takes on a typical value for MOX fuel, somewhat higher than that observed for UOX. This is due in part to the substantial fast fission cross section for thermalnonfissile isotopes such as Pu-238 as well as resonance absorption for the fissile plutoniums. The stronger resonance absorption observed in MOX fuel as compared to UOX can be seen in the resonance escape probability, which takes on a somewhat lower value than the 0.7 - 0.85typical of lattices fuelled with UOX. The thermal utilization also deviates from expected values, for two reasons. First, the benchmark cases disregard fission products, so the substantial thermal capture from these nuclides that develops during the course of a burn is missing. Second, there are no control absorbers, burnable poisons or shim, so the only significant parasitic absorber present is the hydrogen in the moderator. The reproduction factor for fresh MOX fuel is typically somewhat lower than for fresh UOX, because of significant thermal capture in the nonfissile plutonium isotopes, especially Pu-240. Given that somewhat less than three neutrons are produced per thermal fission event, n values of 1.55 to 1.66 imply that only slightly more than half of actinide thermal neutron absorptions lead to fission.

We turn next to the energy dependent flux distribution. This is shown in Figure 6. The averaged fluxes in the fuel pin and moderator/coolant (annular) regions are shown. Several typical features are visible. At highest energies, we see the broad peak in the MeV range representing the fission neutron energy region and the dips in the hundreds of keV through few MeV region caused by oxygen scattering resonances. In the epithermal range, we observe an almost flat region representing a near constant slowing down density. In the lower end of this region, which is characterized by broader resonances in lethargy space, the spectrum is visibly suppressed at several locations. The most notable of these are the lowest-energy resonances in Pu-239 and Pu-240. Students may already know that, in the absence of absorption, the principle of detailed balance requires that the neutron energy spectrum at thermal energies be Maxwellian in shape. This shape is visible in the figures, albeit distorted in the fuel region by the very pronounced effect of the lowest Pu-239 resonance. Finally, since the spectra in both spatial regions are normalized to a common basis, the thermal disadvantage factor ζ may be inferred from the figures. This factor is defined as the ratio of the average thermal flux in the moderator region to that in the fuel; due to strong absorption in the fuel, it is always greater than unity in a reactor. Since MOX pins are especially strong absorbers, and since no shim is present in the moderator, ζ is rather large in this case, ranging from about 1.6 for the fresh configuration down to 1.3 for the depleted fuel.



Figure 6. Neutron Energy Spectra for Fresh (Left) and 60 MWd/kg (Right) Fuel Compositions

Finally, in Figure 7 we present without extensive comment the reactivity coefficients derived by V:BUDS. The fuel temperature (doppler) coefficient assumes a rather typical value, representing increased resonance capture as temperature and thus doppler broadening of resonances increases. V:BUDS computes two moderator coefficients: temperature at constant density and void (varying the density at constant temperature). At this time, V:BUDS does not evaluate the density change that corresponds to a given perturbation in the temperature. The moderator coefficients must not be taken too seriously as the very significant effect of leakage is missing from this infinite-lattice example.



Figure 7. Reactivity Coefficients for Fresh Fuel Composition

We proceed to the time-dependent simulation in which fresh MOX is burned over three 450 day cycles to 48 MWd/kg. As in the NEA benchmark, the burn is conducted at constant power density, which implies that the magnitude of the flux increases with time. For fuel burnup cases such as this, V:BUDS evaluates the neutron balance at user-specified intervals, producing plots analogous to those shown in Figures 4 and 5. These (neutron production and destruction, six factor formula) may be plotted against the time or the cumulative burnup. Additionally, V:BUDS solves the Bateman equations, producing plots of actinide number density or relative concentration versus time or burnup.

We will first consider neutron production and consumption by species. As before, V:BUDS normalizes the results so that the total neutron consumption rate is equal to unity. Figure 8 shows the consumption; note that the y-axis has been set to a logarithmic scale for ease of viewing. The buildup of fission products and to a lesser extent Pu-241 is evident. These take the place of Pu-239 as neutron consumers as that species is depleted. There is no dramatic spectral shift during the course of the burn, as usual for relatively low-burnup MOX fuel. This can be deduced from the nearly constant consumption rate of species with fixed (or nearly fixed) number densities such as U-238 and H in H₂O. A very dramatic shift – from an epithermal to a strongly thermalized spectrum – can be obtained if one implements a very high burnup (> 500 MWd/kg) inert matrix, fertile-free pin cell in a water-moderated assembly. Here one will see a strong increase in the moderating power of the water as the fuel burns out.



Figure 8. Burnup-Dependent Relative Neutron Consumption Rate by Species from Dynamic Calculation

We return to our less exciting example of a traditional MOX pin-cell and consider the neutron production rates shown in Figure 9. The V:BUDS results show that the bulk of fission neutrons are supplied by Pu-239, with Pu-241 playing a more important role late in the lifetime of the fuel. Fast fissions in U-238 and Pu-240 play a minor role throughout.



Figure 9. Burnup-Dependent Relative Neutron Production Rate by Species from Dynamic Calculation

Figure 10 shows the evolution of the six-factor formula terms as the burn proceeds. The burnup benchmark uses a tighter lattice than was true for the earlier example. Additionally, its moderator temperature is higher and density lower. Therefore, the spectrum is harder and the resonance escape probability is decreased to only about 50%: hence, a good deal of epithermal

and fast parasitic absorption in fission products and nonfissile actinides is taking place. Only about two-thirds of neutrons are still produced from thermal fission. K_{eff} decreases throughout the burn, but this figure does not identify a single mechanism producing a majority of the drop in the multiplication factor. Rather, one can only say that over time somewhat fewer fast neutrons induce fast fission, fewer of the fast neutrons that are left reach thermal energies, and fewer thermal neutrons are absorbed in the fuel, and fewer of these actually induce fission. These effects are roughly comparable in magnitude. MOX fuel in general produces a less dramatic burnup K_{eff} shift than does UOX, due in large part to its fertile Pu-240 content. Comparing Figure 9 to an analogous illustration of a UOX burn could be valuable.



Figure 10. Burnup-Dependent Keff and Six Factor Formula Terms from Dynamic Calculation

Finally, we will consider the buildup and depletion of several actinide isotopes. Figure 11 shows the prevalence of four plutonium and four other actinide isotopes as a function of burnup. The dynamics of the system described by the Bateman equations is complex, and we will undertake to qualitatively describe the behavior of a few of the nuclides. Clearly, Pu-239 is the primary fissile fuel for the reactor; during the course of this burn, the rate of capture in U-238 never approaches the rate at which Pu-239 absorbs neutrons, and the Pu-239 is depleted. The situation for Pu-241 is different: Pu-240 capture causes it to be replaced about as quickly as it is consumed. This secular equilibrium cannot be maintained indefinitely: we see that the Pu-240 inventory decreases as its own parent, Pu-239, is consumed.



Figure 11. Evolution of Isotopic Composition for Selected Plutonium (Left) and Other (Right) Actinides

Turning to the minor actinides, we first consider Am-241. Note the apparent discontinuities in its concentration at 16 and 32 MWd/kg. Am-241 is produced by decay of 14.4 year Pu-241; hence, during the downtimes that occur one-third and two-thirds of the way through the burn, it continues to build in while most of the other nuclides shown here remain at roughly constant concentration. Another nuclide with a relatively short half-life (1.7 years) is Cm-242. A noticeable amount of this isotope decays (to Pu-238) during the downtimes. In general, none of the minor actinide species shown here stabilize their concentration during the course of the burn – the rate at which they are produced, whether by neutron capture (in Pu-242 for Am-243, Am-241 for Cm-242 and Am-243 for Cm-244) or by decay (of Pu-241 for Am-241), remains greater than the rate at which they themselves capture neutrons or decay. This in fact represents one of the obstacles of MOX use: producing a unit of energy from MOX fuel creates many times more Am and Cm than is the case for UOX fuel. Certain of the Am and Cm isotopes are quite radioactive and complicate spent fuel handling and disposal.

5. Conclusions

In this paper, we have presented a new tool for the rapid simulation and visualization of the reactor physical and burnup properties of nuclear fuel. This tool, V:BUDS, utilizes a simplified pin-cell representation of the fuel and implements a multigroup collision probability model to obtain the distribution of neutrons in space and energy. V:BUDS is bundled with custom cross section libraries assembled from the ENDF/B-VI nuclear data files. As such, it has been shown to simulate a wide variety of materials, geometries and fuel burnup scenarios with reasonable accuracy. It features a user-friendly GUI and graphical output in the form of MATLAB plots.

Learners endeavoring to master the field of reactor physics are confronted with a very large space of inputs that can be varied – temperature, geometry, fuel composition as quantified by the prevalence of dozens of individual actinide isotopes, and others. The process of understanding the sensitivity of a desired output to variations in each of these inputs is largely one of trial and error that must be conducted by each student. While V:BUDS was not originally developed as a teaching tool, its utility for pedagogy rests upon its ability to expedite and simplify this lengthy intuition-building process.

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