

Burnup Simulations of an Inert Matrix Fuel Using a Two Region, Multigroup Reactor Physics Model

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Abstract

Determining the time dependent concentration of isotopes in a nuclear reactor core is of fundamental importance to analysis of nuclear fuel cycles and the impact of spent fuels on long term storage facilities. We present a fast, conceptually simple tool for performing burnup calculations applicable to obtaining isotopic balances as a function of fuel burnup. The code (VBUDS: visualization, burnup, depletion and spectra) uses a two region, multigroup collision probability model to determine the energy dependent neutron flux and tracks the buildup and burnout of 24 actinides, as well as fission products. The model has been tested against benchmarked results for LWRs burning UOX and MOX, as well as MONTEBURNS simulations of zirconium oxide based IMF, all with strong fidelity. As an illustrative example, VBUDS burnup calculation results for an IMF fuel are presented in this paper.

KEYWORDS: *Burnup, Transmutation, Reactor Physics, Inert Matrix Fuels*

1. Introduction

Fuel burnup calculations are of central importance to nuclear fuel cycle systems analysis, yet many of the tools used for such calculations are complex and poorly suited to performing the large number of moderate-fidelity calculations that are required by a fuel cycle simulation or optimization model. We have developed a fast, simplified method for performing burnup simulations that requires a minimum of setup time, and we have implemented it through a MATLAB interface for computational applications. Our reactor physics model (VBUDS: visualization, burnup, depletion and spectra) uses a two region, multigroup collision probability model to determine the energy dependent neutron flux and tracks the buildup and burnout of 24 actinides, as well as fission products.

The applicability of our method rests on the premise that detailed spatial variations in the neutron flux are unimportant provided that average cross sections, $\langle \sigma \rangle$, and fluxes, ϕ_{ave} , can be derived that preserve interaction rates within macroscopic regions of a reactors core [1]. Collision probability theory [2, pp 394] then models the transport of neutrons from region-to-

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region using transmission and escape probabilities. These methods have existed since the early days of reactor physics [3-5] and are applicable to situations where highest-fidelity computation of the spatial variation in the neutron flux is not required.

The overall aim of our approach is to reduce the spatial dependence of the problem to that of only a few regions while preserving the detailed energy spectrum of the neutron field with a reactor's fuel and moderator regions. Such an approach was used in the WIMSD-5 code developed by the British [6] and was intended primarily for static neutronics calculations on thermal reactors. We have extended this approach to consider the time dependence of the spatial and energy dependent neutron flux in a reactor core in a way that is amenable to rapid computation on a PC. Our model requires a simple set of inputs: fuel element geometry and composition, moderator/coolant geometry and composition, reactor geometry, fuel residence time and target discharge burnup.

To date VBUDS has been tested against several benchmarked standards for LWR UOX/MOX that are available from the NEA/OECD [7, 8] and against inert matrix fuel (IMF) burnup calculations that were done using MONTEBURNS [9], all with high fidelity. In this paper we detail burnup simulations conducted with VBUDS on an IMF with high transuranic loading. The beginning and end of life neutron spectra for the fuel are presented along with the burnup dependence of terms in the four-factor formula. The time dependence of selected isotopes that act as neutron sources and sinks are also given, as are burnup calculation results relevant to the study of nuclear fuel cycle strategies.

2. Methodology

VBUDS uses collision probability approximations on a representative unit cell to decouple the spatial and energy dependences of the neutron flux in the neutron transport equation. The energy dependent neutron flux, governed by coupled integral equations for the fuel and moderator/coolant regions is treated by multigroup thermalization methods, and the transport of neutrons through space is modeled by fuel to moderator transport and escape probabilities [1]. For purposes of energy transfer, we preserve the isotropic and linearly anisotropic components of the elastic scattering kernel in the center-of-mass system. To decouple space and energy in the transport equation, we use a simple transport approximation in which scattering devolves into forward and isotropic components.

To model the transport of neutrons between the spatial regions of the fuel and moderator/coolant, an effective cell consisting of a fuel element surrounded by a region of moderator/coolant is constructed. The transport of neutrons between regions is then governed by transmission and escape probabilities, which are themselves functions of energy. By taking the neutron number density in the respective fuel and moderator/coolant regions to be uniform, we may apply the reciprocity theorem and greatly simplify spatial transport computations. The goal is not to accurately model the spatial distribution of neutrons, but instead their energy distribution on which the isotopic balance of a reactor most strongly depends.

VBUDS uses a multigroup formulation to treat neutron energy dependence. The ENDF/B-VI

data were processed using NJOY [10], to yield cross section libraries and self shielding factors at 5 temperatures (300, 600, 900, 1200, 1500 K). Cross sections come bundled with VBUDS for a wide range of potential constituents which include 24 actinide isotopes, oxide, nitride, zirconia, and zirconium hydride fuel forms, cladding and structural materials and a number of common moderators and coolants.

3. Results

As an illustrative case, we consider a LWR burning inert matrix fuel (IMF) with 92 w/o zirconium oxide and 8 w/o minor actinides (MA) and plutonium. The isotopic vector, unit lattice cell and other geometric and material inputs required for the run are described in detail in [11]. To summarize, the simulation utilizes a right cylindrical lattice with fuel pin radius 0.41 cm, pitch 1.27 cm and clad thickness 0.065 cm. A 3x3 pin array would in practice contain one IMF and eight UOX pins. The burnup calculation was carried out at constant power with a fuel residence time of 1611 effective full power days. The discharge IMF burnup, 550 MWd/kg, was a derived parameter. It was obtained through a simple estimate of the infinite-medium multiplication factor of the core, assuming a three-batch fuel management scheme. A discharge burnup of 550 MWd/kg was found to be the value at which a core containing one part in three of fuel having undergone one, two and three irradiation cycles achieved a k_{inf} of about 1.03. This approach, while crude, is in widespread use for first-order cycle length estimates and our discharge burnup result compares well to that used in [11].

The transuranics used in the IMF are drawn from 30 year cooled spent UOX burned to 45 MWd/kg. Our IMF scenario envisions the separation of all transuranics via a UREX process from the 30 year cooled UOX, followed by the fabrication of IMF from the recovered TRUs. Recovered uranium and fission products would be stored pending disposal, as would spent IMF fuel pins. The irradiated IMF isotopic concentrations discussed here have been benchmarked against MONTEBURNS [9] calculations and the results produced by VBUDS showed a very strong correlation [1].

We outline the principal results of the VBUDS burnup calculation and connect them to the repository impact of IMF use. The neutron spectrum averaged over the IMF fuel region is shown in Fig. 1 along with the coefficients of the four factor formula, Fig. 2. Recall that according to the four factor formula the infinite medium multiplication factor is the product of the four neutron balance coefficients shown in the figure. The four factor formula is described in most introductory textbooks [2, pp 283]. In Fig.2, the individual terms and multiplication factor are computed in the absence of adjustable control absorber.

Figure 1: Neutron spectrum at charge and discharge. The residence time of the fuel in the simulations is 1611.11 days at full power. Fuel burnup at discharge is 550 [MWd/kg IHM]. The spectrum can be seen to have softened considerably at discharge, owing to the burnout of Pu which strongly captures thermal neutrons. The vertical axis is on an arbitrary scale, the horizontal scale is in eV on a log scale.

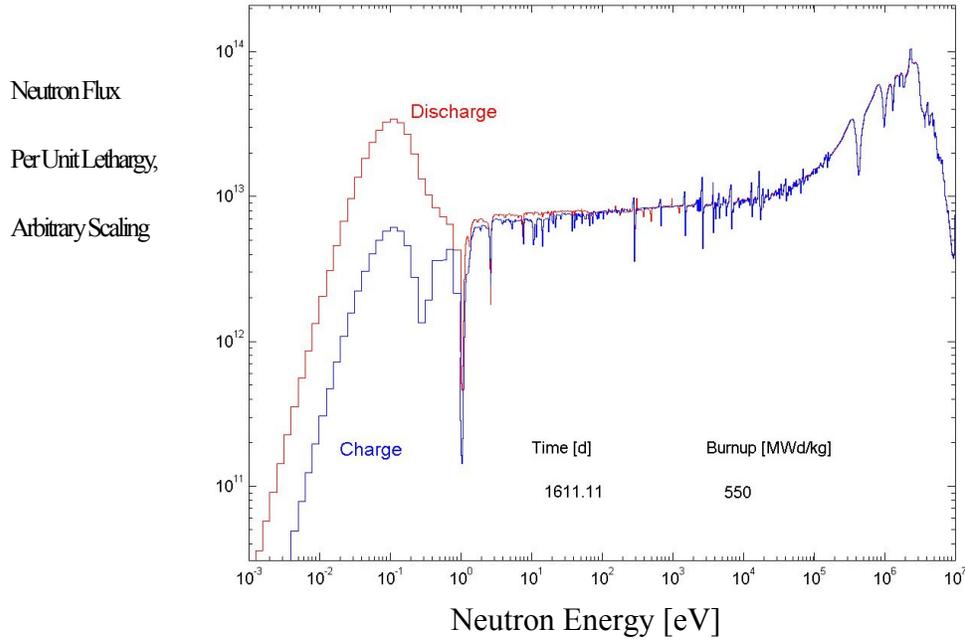
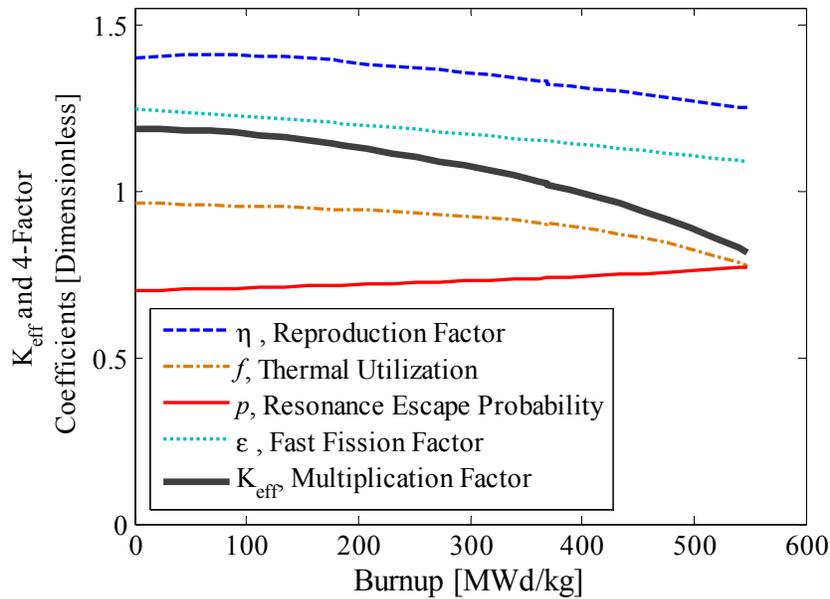


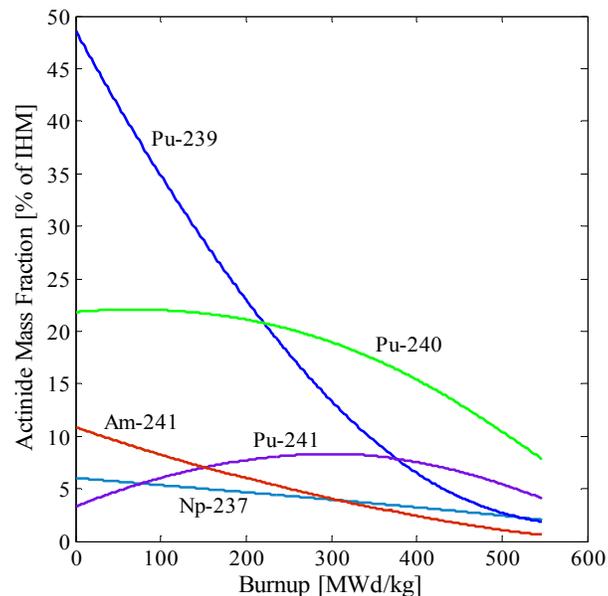
Figure 2: Parameters of the four factor formula as a function of fuel burnup. The neutron reproduction, thermal utilization, resonance escape probability, fast fission, and multiplication factors are shown as a function of fuel burnup. The simulation was done assuming an infinite lattice and the leakage factors are therefore equal to one.



It can be seen from Fig. 1 that the neutron energy spectrum softens significantly during irradiation. This is expected since the high TRU content of a fresh IMF leads to a short neutron mean free path even at epithermal energies. As the most strongly absorbing TRUs are fissioned (or otherwise transmuted) the effective moderating power of the pin-cell assembly increases. This evolution can also be seen in Fig. 2 where the burnup reactivity swing is revealed to be strongly influenced by the fuel utilization. The decline in the reproduction factor, defined as the number of neutrons produced per neutron absorbed in the fuel, reflects the burnout of fissile isotopes and the general increase in the capture to fission ratio that takes place during burnup.

We show the concentration of actinides of greatest interest in Fig. 3. Of the initial Pu-239, and Am-241 present in the fresh IMF more than 95% and 90% are transmuted, respectively. The resultant Pu vector, dominated by Pu-240, is highly degraded from the standpoint of a potential proliferation [12]. The long-term prevalence of Np-237 is reduced by approximately a factor of two, which will be of benefit in reducing the long-term radiological load to be borne by a repository.

Figure 3: Concentration of selected actinide isotopes during burnup. Breeding of Pu-241 from fertile Pu-240 plays an important role in supporting the reactivity of the fuel. The downside of this is that the fuel remains a net producer of this precursor to Am-241.



Figs. 4 and 5 show the neutron production and consumption rates, normalized to unit total neutron consumption, for the unit cell. Although substantial quantities of a number of actinide isotopes are bred during irradiation, neutron multiplication in the cell depends on the two principal plutonium isotopes throughout the irradiation period. The importance of Pu-241, bred from Pu-240, in sustaining criticality is clearly evident. A plutonium vector containing more Pu-239, for instance as part of a weapons plutonium disposition strategy, would result in a much steeper burnup reactivity swing and more intensive use of burnable poison to maintain a smooth power profile.

Figure 4: Fission neutron production rate by fissioning isotope. The total is normalized to a unit consumption rate in the absence of adjustable control absorber.

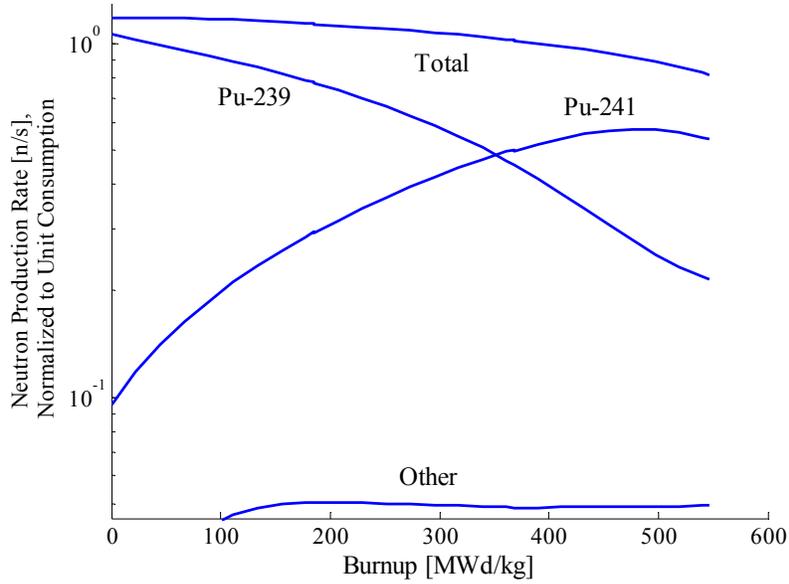
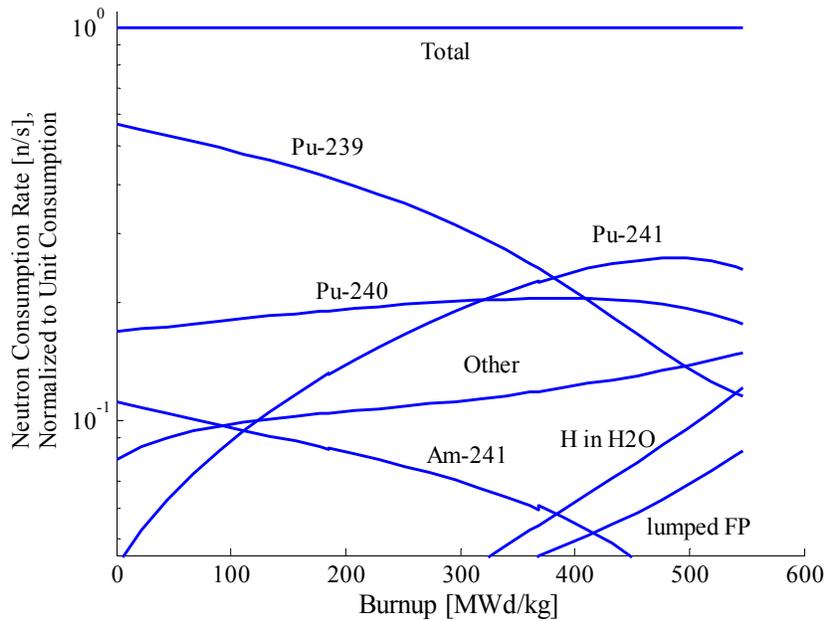


Figure 5: Neutron consumption rate by consuming isotope. Normalized to unity, discounting adjustable control absorber.



Neutron consumption, in the absence of adjustable control absorber, is dominated by absorption in the three principal plutonium isotopes. Although IMF irradiation yields a slight net

positive Pu-242 production, this isotope does not strongly affect the neutron balance. One effect of the softening spectrum – the increase in the hydrogen capture rate – can clearly be seen. As an aside, the production and destruction rates can easily be converted to one group cross sections for use in a more detailed ORIGEN2.2 [13] burnup calculation that would, for instance, yield the fission product isotopic distribution in full detail. In fact, this ORIGEN calculation was performed to obtain the repository impact results we turn to next.

The capacity of a repository, like Yucca Mountain, will be substantially governed by the decay heat production of the waste being interred. In the longer term (on the order of the mean time to failure of waste packages or greater) the radiotoxicity or the specific activity of the waste would become relevant to fission product and heavy metal transport calculations. Hence, we plot two metrics for two scenarios: 1) direct disposal of the unprocessed 45 MWd/kg UOX fuel, and 2) disposal of waste that would be associated with the IMF strategy, namely the IMF SNF, fission product bearing HLW from reprocessing of the UOX fuel and (for consistency) the uranium recovered from processing of the UOX.

Fig. 6 shows the radioactivity of the waste for the two scenarios, for time scales extending to 1 million years, while Fig. 7 displays the decay power over a 10,000 year period. It is likely that the repository capacity will be fixed by the decay power of the waste integrated over a time period commencing when active cooling of the repository ceases and extending perhaps 1500 years in the future [14, p. 3]. The activities and heat loads are normalized on the basis of equivalence of energy production between the direct disposal and IMF scenarios.

Figure 6: Activity [Ci] of repository-bound material, direct disposal vs. IMF. The activities are computed on the basis of equivalent energy produced in the reactor. In other words, 1.159 kg of UOX, irradiated to 45 MWd/kg, produces the same amount of energy as 1.0 kg of UOX irradiated to 45 MWd/kg plus 0.0130 kg of IMF burned to 550 MWd/kg. Note that 1.0 kg of the spent UOX used in this study, when reprocessed, yields 0.0130 kg of transuranics. For reasons of consistency, the 0.9401 kg of uranium recovered from the 1.0 kg of reprocessed UOX is included in the calculation of IMF-scenario activity. Hence, since a number of uranium isotopes are important contributors to the activity in the very long term, for decay times of greater than 100,000 years there is little difference between the two scenarios.

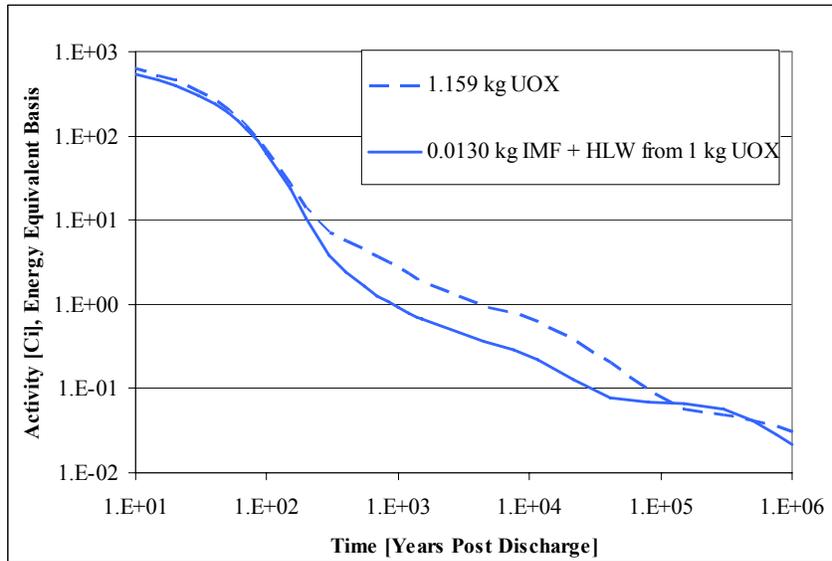
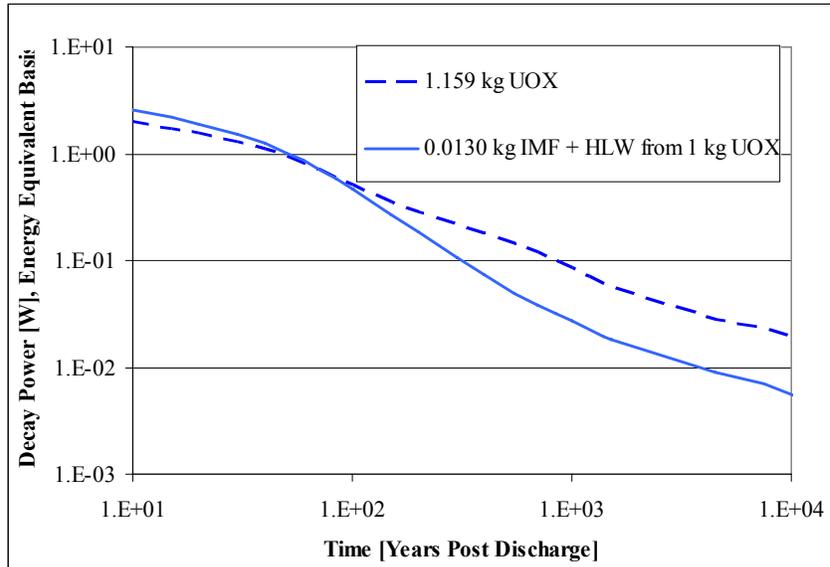


Figure 7: Decay power [W] of repository-bound material, direct disposal vs. IMF. The decay power is computed on the basis of equivalent energy production, following the reasoning given in the preceding figure caption. Medium and long term decay power is seen to be substantially reduced if the IMF strategy is pursued. The reduction at 1500 years of decay is a factor of three.



4. Conclusions

The VBUDS run time for the burnup calculations was on the order of seconds which is considerably shorter than would be required for simulations done with other reactor physics codes. Comparison of VBUDS simulations with available benchmarks for LWRs burning MOX and UOX as well as comparison of results for the IMF simulation with those obtained using MONTEBURNS indicate a high degree of reliability for the data produced by VBUDS [1, 15].

To allow for the automated generation of fuel cycle scenario results such as time-dependent heat load and activity of repository waste, work is ongoing to incorporate VBUDS into a full fuel cycle simulation package.

Acknowledgements

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