Argonne NATIONAL LABORATORY

ANL-11/34

Conceptual Design of Minor Actinides Burner with an Accelerator-Driven Subcritical System

Nuclear Engineering Division

About Argonne National Laboratory
Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC under contract DE-AC02-06CH11357. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne, see www.anl.gov.

Availability of This Report
This report is available, at no cost, at http://www.osti.gov/bridge. It is also available on paper to the U.S. Department of Energy and its contractors, for a processing fee, from:

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
phone (865) 576-8401
fax (865) 576-5728
reports@adonis.osti.gov

Disclaimer
This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor UChicago Argonne, LLC, nor any of their employees or officers, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of document authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof, Argonne National Laboratory, or UChicago Argonne, LLC.

ANL-11/34

Conceptual Design of a Minor Actinides Burner with an Accelerator-Driven Subcritical System

by
Yan Cao and Yousry Gohar
Nuclear Engineering Division, Argonne National Laboratory

September 2011

Conceptual Design of a Minor Actinides Burner with an Accelerator-Driven Subcritical System

Contents

Page

ABSTRACT 1

2 SPALLATION NEUTRON SOURCE DESIGN 3

3 SUBCRITICAL FISSION BLANKET DESIGN 4

3.1 FISSION BLANKET NEUTRON MULTIPLICATION 4

3.2 FISSION BLANKET ENERGY MULTIPLICATION 5

3.3 INITIAL FUEL INVENTORY AND GEOMETRICAL SIZE OF FISSION BLANKET 5

4 FUEL BURNUP ANALYSIS 6

4.1 AM-241 TRANSMUTATION 6

4.2 BURNUP SIMULATIONS: TEST CASE 8

4.3 BURNUP SIMULATIONS: CASES I-III 8

5 SUMMARY 11

REFERENCES 13

APPENDIX B: COMPUTER SCRIPT CODES 37

B.1 PYTHON JOB SCRIPT TO CALCULATE FEED FACTOR *F* OF APPENDIX A 37

B.2 PYTHON JOB SCRIPT TO ADJUST FEED FACTOR *F* 45

B.3 SHELL SCRIPT TO RUN MCB5 CODE 47

Figures

Page

Figure 1. ADS system schematic representation (White: proton beam current channel; Green: LBE target/coolant; Blue: HT-9 wall; Yellow: LBE fuel blanket; Red: graphite). 19

Figure 2. LBE total energy deposition as function of target length for various proton energies. 19

Figure 3 Fission blanket infinite neutron multiplication as a function U-Pu concentration in actinide mixture for various actinide concentrations in LBE fuel carrier of blanket. 20

Figure 4 Fission blanket effective neutron multiplication with 7% actinides in LBE fuel carrier as a function of plutonium concentration in actinide mixture and corresponding total power in ADS system obtained by 1GeV proton beam with 25 MW beam power at each k_{eff} value. 20

Figure 5 Fission blanket effective neutron multiplication with 2% actinides consisting of 50% plutonium and 7% actinides consisting of 27.2% plutonium in LBE fuel carrier as a function of graphite reflector thickness. 21

Figure 6 Fission blanket neutron spectra with 7% actinides consisting of 27.2% plutonium fraction in LBE fuel carrier for various graphite reflector thicknesses. 21

Figure 7 Minor actinide inventories in fission blankets with 0.98 effective neutron multiplication factor and their volumes as a function of plutonium concentration in actinide mixture for three blanket configurations with 5, 7, and 10% actinide concentration in LBE fuel. 22

Figure 8 Am-241(n,g)Am-242g branching ratios from Mann & Schneter calculation, ENDF/B-VI.8, –VII.0 nuclear data files, and CINDER90 library. 22

Figure 9 Effective neutron multiplication factor and Am-242m concentration in test blanket for first 5 burnup years driven by 25 MW beam power using 1 GeV protons. 23

Figure 10 Actinide fuel compositions in test blanket for first 5 burnup years driven by 25 MW beam power using 1 GeV protons. 23

Figure 11 Effective neutron multiplication value before and after each fuel burnup time step for the three fission blanket configurations of Table IV. 24

Figure 12 Actinides and LLFPs annual feeding rates at end of each burnup step for blanket configuration with 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides. 24

Figure 13 Actinides and LLFPs annual feeding rates at end of each burnup step for the blanket configuration with 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides. 25

Figure 14 Actinides and LLFPs annual feeding rates at end of each burnup step for the blanket configuration with 10% actinide concentration in LBE and 20% plutonium concentration in actinides. 25

Figure 15 Total actinides and LLFPs feed at end of each burnup step for blanket configuration with 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides. 26

Figure 16 Total actinides and LLFPs products feed at end of each burnup step for blanket configuration with 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides. 26

Figure 17 Total actinides and LLFPs feed at end of each burnup step for blanket configuration with 10% actinide concentration in LBE and 20% plutonium concentration in actinides..... 27

Figure 18 Actinides, U-Pu, and MAs transmutation rates for three blanket configurations of Table IV. 27

Figure 19 Consumption of actinide isotopes during first 10 burnup years for blanket configuration with 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides. 28

Figure 20 Consumption of actinide isotopes during first 10 burnup years for blanket configuration with 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides. 28

Figure 21 Consumption of actinide isotopes during first 10 burnup years for blanket configuration with 10% actinide concentration in LBE and 20% plutonium concentration in actinides..... 29

Figure 22 Actinide isotopic compositions during first 10 burnup years for blanket configuration 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides..... 29

Figure 23 Actinide isotopic compositions during first 10 burnup years for blanket configuration 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides..... 30

Figure 24 Actinide isotopic compositions during first 10 burnup years for blanket configuration 10% actinide concentration in LBE and 20% plutonium concentration in actinides..... 30

Figure 25 Annual transmutation rates of actinide isotopes and LLFPs isotopes during first 10 burnup years for blanket configuration 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides. 31

Figure 26 Annual transmutation rates of actinide isotopes and LLFPs isotopes during first 10 burnup years for blanket configuration 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides. 31

Figure 27 Annual transmutation rates of actinide isotopes and LLFPs isotopes during first 10 burnup years for blanket configuration 10% actinide concentration in LBE and 20% plutonium concentration in actinides. 32

Figure 28 Actinides, U-Pu, and MAs inventories at each time-step during first 10 burnup years for the three blanket configurations of Table IV..... 32

Figure 29 LLFPs consumption during first 10 burnup years for blanket configuration with 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides..... 33

Figure 30 LLFPs consumption during first 10 burnup years for blanket configuration with 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides..... 33

Figure 31 LLFPs consumption during first 10 burnup years for blanket configuration with 10% actinide concentration in LBE and 20% plutonium concentration in actinides..... 34

Tables

Page

Table I. Main parameters of LBE target designs. 15

Table II. Physical properties of ADS system materials..... 15

Table III. Energy multiplication of 25 MW proton beam power with 1 GeV protons from various fission blanket configurations. 16

Table IV. Three fission blanket configurations with 0.98 k_{eff} and MA inventory ≤ 10 tons. 16

Table V. Annual feeding rates, annual transmutation rates at tenth year of fuel burnup, and total transmutation after first ten burnup years for the three fission blanket configurations in Table IV. 17

Table VI. Total feed, total production from fission reactions, and total transmutations of LLFPs after first ten burnup years for the three fission blanket configurations in Table IV. 18

Table VII. Transmutation rates and effective half-lives of LLFPs after first ten burnup years for the three fission blanket configurations in Table IV. 18

Conceptual Design of a Minor Actinides Burner with an Accelerator-Driven Subcritical System

Abstract

In the environmental impact study of the Yucca Mountain nuclear waste repository, the limit of spent nuclear fuel (SNF) for disposal is assessed at 70,000 metric tons of heavy metal (MTHM), among which 63,000 MTHM are the projected SNF discharge from U.S. commercial nuclear power plants though 2011. Within the 70,000 MTHM of SNF in storage, approximately 115 tons would be minor actinides (MAs) and 585 tons would be plutonium. This study describes the conceptual design of an accelerator-driven subcritical (ADS) system intended to utilize (burn) the 115 tons of MAs.

The ADS system consists of a subcritical fission blanket where the MAs fuel will be burned, a spallation neutron source to drive the fission blanket, and a radiation shield to reduce the radiation dose to an acceptable level. The spallation neutrons are generated from the interaction of a 1 GeV proton beam with a lead-bismuth eutectic (LBE) or liquid lead target. In this concept, the fission blanket consists of a liquid mobile fuel and the fuel carrier can be LBE, liquid lead, or molten salt. The actinide fuel materials are dissolved, mixed, or suspended in the liquid fuel carrier. Therefore, fresh fuel can be fed into the fission blanket to adjust its reactivity and to control system power during operation.

Monte Carlo analyses were performed to determine the overall parameters of an ADS system utilizing LBE as an example. Steady-state Monte Carlo simulations were studied for three fission blanket configurations that are similar except that the loaded amount of actinide fuel in the LBE is either 5, 7, or 10% of the total volume of the blanket, respectively. The neutron multiplication factor values of the three configurations are all approximately 0.98 and the MA initial inventories are each approximately 10 tons. Monte Carlo burnup simulations using the MCB5 code were performed to analyze the performance of the three conceptual ADS systems. Preliminary burnup analysis shows that all three conceptual ADS systems consume about 1.2 tons of actinides per year and produce 3 GW thermal power, with a proton beam power of 25 MW. Total MA fuel that would be consumed in the first 10 years of operation is 9.85, 11.80, or 12.68 tons, respectively, for the systems with 5, 7, or 10% actinide fuel particles loaded in the LBE. The corresponding annual MA fuel transmutation rate after reaching equilibrium at 10 years of operation is 0.83, 0.94, or 1.02 tons/year, respectively. Assuming that the ADS systems can be operated for 35 full-power years, the total MAs consumed in the three ADS systems are 30.6, 35.3, and 37.2 tons, respectively. For the three configurations, it is estimated that 3.8, 3.3, or 3.1 ADS system units are required to utilize the entire115 tons of MA fuel in the SNF inventory, respectively.

1 Introduction

In U.S. Department of Energy (DOE) environmental impact studies of the Yucca Mountain nuclear waste repository [1], the limit of spent nuclear fuel (SNF) to be disposed of is 70,000 metric tons of heavy metal (MTHM), among which would be 63,000 MTHM of projected SNF discharge from U.S. commercial nuclear power plants through 2011. Compositions of the discharged spent nuclear fuel from the light water reactors (LWRs) differ from one reactor unit to another due to differences in initial fuel composition, irradiation history, and post-irradiation processing steps (i.e., cooling-time conditions) [2]. However, the total amount of transuranics is only ~1% of the LWR discharged fuel.

This report describes the proposed accelerator-driven subcritical (ADS) systems that would burn the transuranics of the discharged SNF. Performances of these systems are functions of initial fuel compositions and fuel feed compositions during operation. Argonne National Laboratory (ANL) has performed a study to define the average composition of the LWR-discharged SNF [2]. Assuming a 0.99995 uranium removal fraction, the SNF consists of ~84% plutonium, ~5.6% neptunium, and ~10.6% americium. Curium isotopes are less than 0.2%. In other words, the 70,000 MTHM SNF contain ~115 tons of minor actinides (MAs) and 585 tons of plutonium. The objective of this study is to design a system that would burn the 115 tons of MAs contained within the 70,000 tons of discharged SNF.

The ADS system consists of a subcritical assembly driven by a spallation neutron source and a radiation shield to reduce the dose to an acceptable level. The spallation neutron target is placed at the center of the system and is surrounded by a cylindrical fission blanket. In this study, graphite is chosen as the reflector material, as shown in Figure 1. The LBE target design of these studies is presented in the next section, followed by steady-state Monte Carlo simulations to define the main parameters of the three fission blanket configurations. Finally, Monte Carlo burnup analyses for these conceptual configurations show the effectiveness of the system for transmuting the MAs.

Use of ADS systems has been discussed in closed-fuel-cycle studies for disposing of SNF in [3,4] due to the potential advantage of using external neutrons from spallation targets, the enhanced safety features of subcritical assemblies, and the flexibility of loading MA fuel in the subcritical assembly. Most of the previous studies adopted the traditional solid fuel form to utilize the gained experience from operating fission power reactors [5-7]. This approach requires the development of several new technologies, i.e., developing and testing new fuel forms loaded with MAs, modifying or replacing current fuel reprocessing techniques to accommodate the new fuel forms containing MAs, and developing extra multistep fuel reprocessing techniques to reduce fuel losses. All of these developments and tests are time-consuming and add significant extra costs. The studies in this report focus on examining the concepts of utilizing mobile fuel forms. The benefits of mobile fuel can be realized immediately as eliminating the necessity of developing new solid fuel forms, easing the burden of the radiation damage in the materials for deeper fuel burnup, and reducing the number of fuel-reprocessing steps after fuel irradiation.

In the mobile fuel concept, the actinide fuels are dissolved, mixed, or suspended in a liquid fuel carrier. The fuel materials can form compounds or exist as suspended micro-particles in the liquid fuel carrier. Therefore, batch or continuous feed operation is feasible, stabilizing the reactivity of the subcritical assembly and controlling the system power. The liquid fuel carrier, based on the past research studies [8, 9], can be either liquid metals, i.e., lead-bismuth eutectic (LBE) or liquid lead, or molten salts, i.e., FLIBE, other fluorides, or chlorides. In this study, LBE is used because of its excellent neutron characteristics and low melting point (397 K). The neutronics characteristics of molten lead are similar to those of LBE in terms of neutron moderation and absorption. The use of lead avoids the buildup of Po-210 and is less corrosive than LBE; however, it has a higher melting point of ~600 K.

2 Spallation Neutron Source Design

In the ADS system design, the spallation target provides the neutron source to operate the subcritical assembly and serves as the interface between the accelerator and the subcritical blanket. A highly detailed target design that utilizes LBE as the target material was designed at ANL in the early 2000s [10]. In this design, physics, thermal-hydraulic, and structure analyses have been iterated to satisfy the engineering constraints required for a safe system. The 24 kJ/cm^2-s energy deposition limit imposed on the target's front window surface leads to a satisfactory target window design and an acceptable operating lifetime. An average velocity limit of 2 m/s is imposed on the LBE coolant to minimize erosion and corrosion of the structural materials.

To minimize design time and effort in this study, the above engineering design was adopted. The geometrical configuration of the new design is scaled to satisfy the two constraints imposed on the design. Therefore, with simple algebra calculations, Table 1 lists the key parameters of the target design for 25 MW beam power with 1 GeV protons compared with the earlier ANL design for 5 MW beam power with 600 MeV protons.

It is well known that in the spallation process, more neutrons can be generated with higher-energy protons. However, studies have shown that the number of generated neutrons normalized to the beam power saturates as the proton energy exceeds 1 GeV [11]. In addition, as shown in Figure 2, the Monte Carlo simulations show that the 1 GeV proton stops after travelling ~62 cm into the LBE target and deposits 99.8% of its energy. However, the 2 GeV proton does not stop before 147 cm and requires about 80 cm to deposit 99% of its kinetic energy. To maintain the compactness of the ADS system as much as possible, proton beam energy was set at 1 GeV, and the neutron target region was designed with a cylindrical shape of 70 cm diameter and 70 cm height.

3 Subcritical Fission Blanket Design

In these preliminary analyses, the fission blanket has a cylinder geometry that surrounds the neutron target. The blanket is a homogeneous zone with actinide fuels either dissolved in LBE or as fuel particles suspended in LBE to form a slurry. Table II lists some of the physical properties of the materials utilized in the analyses. The mass density of LBE at 900 K is calculated on the basis of OECD handbook data [12]. The actinide fuel is the recommended composition of the ANL report [2], which is the LWR discharged fuel after 25 years cooling time and the removal of 99.995% of the uranium.

Although it is known that the solubility of the actinide fuels in LBE is low and increases with temperature, detailed experimental or analytical data in the literature are difficult to find. According to the phase diagram [13], actinide solubilities in LBE at 900 K (mainly Pu, Np, and Am) are estimated at less than 2%. Experimental work by Hahn showed that LBE can contain reduced uranium oxide particles in concentrations as high as 13% [8] to form steady slurries.

3.1 Fission Blanket Neutron Multiplication

The first analytical step is to determine the neutron multiplication factor as a function of actinide concentration in LBE. Five different actinide concentrations in LBE are considered in the simulations: 2, 3, 5, 7, and 10%. In the 2% and 3% cases, it is assumed that the actinide fuel dissolves into the LBE and that the atomic percentages of the total actinide fuel atoms are utilized. In the 5-10% cases, the fission blanket zone is filled with slurry and the volume fraction of the suspended actinide oxide particles in the slurry is utilized.

In addition, neutron multiplication of the fission blanket depends on the fuel compositions in the solution or in the fuel particles. Because the principal aim is to burn MAs, the plutonium concentration is minimized. During the simulations, the isotopes in the discharged SNF vector shown in Table II are grouped into two parts: (a) the plutonium part, including all the plutonium and uranium isotopes; and (b) the MA part, including all the neptunium, americium, and curium isotopes. The major isotopes in the MA part, i.e., Np-237 and Am-241, are all fertile in the thermal neutron spectrum and have small fission cross sections in the fast neutron spectrum. The plutonium part, mainly Pu-239, is utilized to boost the neutron multiplication of the fission blanket.

Figure 3 shows the neutron multiplication factors of the fission blankets with various actinide fuel concentrations and plutonium concentrations. Simulation confirms that the neutron multiplication factor increases as plutonium concentration increases in the actinide fuel. The results show that with higher actinide concentrations loaded in the system, the neutron multiplication factor increases. In addition, simulation indicates that the actinide fuels should contain at least 40 at% plutonium for the case with 2% actinides in order to achieve a neutron multiplication factor of 0.98. The plutonium concentration required to achieve high neutron multiplications decreases as more actinide fuels are loaded in LBE, i.e., a minimum ~13 at% plutonium is required in the

fission blanket to achieve the neutron multiplication factor of 0.98 in the case of 10% actinide in LBE.

3.2 Fission Blanket Energy Multiplication

In fission reactors, the actinide fuel consumption rate is determined by the fission power generated in the system. For an ADS system, the fission power generated in the blanket is often proportional to the accelerator beam power and the neutron multiplications:

$$P \propto k/(1-k), \tag{1}$$

where k is the source neutron multiplication factor and is slightly different than the traditional fission source neutron multiplication factor k_{eff} of the ADS system.

Figure 4 shows the fission power generated in the ADS system for a specific fission blanket design at various neutron multiplication values. In the simulations, actinide fuel concentration is set at 7%, and the height and the diameter of the cylindrical fission blanket are each 3.0 m. The neutron multiplication factor is adjusted by changing the plutonium concentration in the actinide fuel particles. According to this figure, the neutron multiplication factor of the fission blanket should be as high as ~0.98 in order to obtain 3 GW thermal power with 25 MW proton beam power when using 1 GeV protons.

In addition, the Monte Carlo simulation results in Table III show that the energy multiplication factors are all very similar for the various ADS system configurations if the fission blankets have a similar k_{eff} ~0.98. Therefore, in the remainder of this report, the neutron multiplication factor of the fission blanket is set to ~0.98 to obtain 3 GW thermal power with a 25 MW proton beam.

3.3 Initial Fuel Inventory and Geometrical Size of Fission Blanket

In an actual fission blanket configuration, the amount of actinide or plutonium required to achieve the neutron multiplication factor of 0.98 is greater than that suggested in Figure 3 due to neutron leakage. The use of a graphite reflector around the fission blanket increases its neutron multiplication. Figure 5 shows that for two specific configurations, k_{eff} increases when a graphite reflector is utilized. The neutron multiplication and the neutron spectrum in the fission blanket will change slightly if the reflector thickness is increased from 150 cm to 250 cm, as shown in Figures 5 and 6. Therefore, in the remainder of this report, graphite reflector thickness is set to 250 cm to reduce neutron leakage from the fission blanket.

Figure 7 shows plutonium concentrations, percentages of actinide fuel loaded in LBE, total MA inventories in the fission blanket, and sizes of the fission blanket required

for the various configurations to achieve a k_{eff} of about 0.98. For a specific fission blanket configuration, the more actinide fuel that is loaded into the LBE, the lower the plutonium concentration that is required in the fuel materials.

The initial MA inventory loaded in a fission blanket is constrained by the SNF processing capacity and the time difference between the start of the SNF processing and the first ADS system operation. If the 70,000 MTHM SNF can be processed within 35 years, about 13 tons of MAs will be available within 4 years to start the first ADS system. Figure 7 can be used to select the desired configuration to satisfy different engineering requirements and to have an acceptable MA inventory.

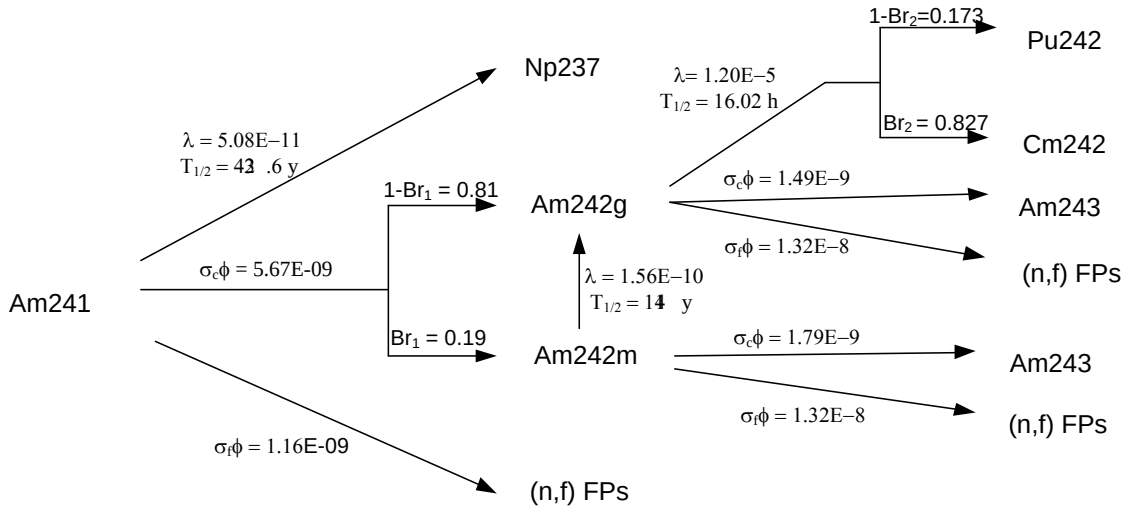
If the fission blanket volume is set to ~20 m^3, the results of Figure 7 show that the configuration with 7% actinide and 27.2% plutonium concentrations has a 0.98 neutron multiplication factor. The volume of this fission blanket is 20.4 m^3 and the weight of MAs loaded in the blanket is 10.0 tons. It is possible to choose different configurations by changing the actinide concentration in the LBE. Other configurations can be defined on the basis of the results of Figure 7. A fission blanket design with 5% actinides and ~36% plutonium concentrations and a fission blanket volume of ~20.4 m^3 provides the same effective neutron multiplication factor of 0.98 with the initial MA loading of ~10 tons. Table IV lists three configurations for the fission blanket based on the Monte Carlo simulation results. These configurations are used in the next step to perform burnup analyses.

4 Fuel Burnup Analysis

As discussed in the previous section, the actinide fuel consumption rate is defined by the fission power generated in the system. For a 3 GW system, the amount of actinides consumed annually is 1.2 tons. During that operation, the neutron multiplication factor of the fission blanket decreases due to the consumption of the fissile materials. However, this is not always the case for an ADS system designed to consume MAs containing a high concentration of Am-241 isotope and a low concentration of plutonium isotopes. The remainder of this section discusses the details of the burnup analyses.

4.1 Am-241 Transmutation

In the ADS system, most of the Am-241 atoms can either be fissioned or transmuted to the fissile isotopes Am-242g or Am-242m through neutron capture, as shown in the diagram below. The various reaction rates are calculated for a fission blanket design with 0.98 k_{eff} and 3 GW thermal power output.



Apparently, as shown in the above diagram, the Am-242g has a short half-life of 16.02 h that leads to its decay constant $\lambda >> \sigma\phi$. Thus, the majority of the Am-242g produced from the Am-241 neutron capture in the system decays quickly to the fertile isotopes Pu-242 or Cm-242. At the same time, the Am-242m has a relatively long half-life of 141 y. Its decay constant is one or two orders of magnitude lower than the calculated neutron capture and fission rates. Thus, the Am-242m isotope will be consumed mainly by fission. A small amount is transmuted to Am-243, and only a very small fraction of Am-242m will decay to the Am-242g. The Batemann equation for the Am-242m isotope is

$$\frac{dN^{Am242m}}{dt} = f^{Am242m} + \left\langle (1-Br_1)\sigma_r^{Am241}\phi \right\rangle N^{Am241} - \left(\lambda^{Am242m} + \left\langle \sigma_r^{Am242m}\phi \right\rangle + \left\langle \sigma_f^{Am242m}\phi \right\rangle\right) N^{Am242m}. \quad (2)$$

The solution of Eq. 2 shows that the Am-242m concentration increases during the first few years of operation after startup due to the high level of Am-241 in the fission blanket.

The maximum amount of Am-242m accumulated in the system is sensitive to the branching ratio of Am-241 neutron capture to Am-242m, and its buildup determines the change of the neutron multiplication factor of the system. However, unlike some of the other branch ratios, i.e., Br_2, which is a fixed number, the branch ratio Br_1 is an energy-dependent function and has very few experimental data points. Significant inconsistencies also exist among current neutron cross section libraries [14]. The ENDF/B-VII nuclear data files have improved this branching ratio based on new differential data and integral measurements [15]. The MCB5 Monte Carlo burnup code [16] utilizes a set of very old analytical data calculated by Mann and Schenter [17]. In the MCNPX code [18], this branch ratio is calculated on the basis of macroscopic cross sections embedded in the CINDER library. As shown in Figure 8, those values are

significantly different from one another at various energy groups. In this report, all of the Monte Carlo burnup simulations are performed by using the MCB5 code, the library for the Am-241 branch ratios is taken from ENDF/B-VII nuclear data files, and all the numerical simulation results are based on the improved ENDF/B-VII libraries.

4.2 Burnup Simulations: Test Case

Before the fuel burnup simulations were performed for the three cases listed in Table IV, a test case was first simulated utilizing the MCB5 code to study buildup of Am-242m in the system. The test case begins with a fission blanket configuration having a low neutron multiplication factor so as to examine the reactivity increase during fuel burnup. Actinide fuel concentration is 7%. The plutonium concentration in the fuel is 22%, to achieve ~0.90 k_{eff} at the beginning of fuel burnup. The fission blanket is driven by 25 mA proton beam (25 MW beam power), and the burnup time-step is 180 days.

The Monte Carlo simulation results shown in Figure 9 confirm that the amount of Am-242m isotope increases in the fission blanket, reaching its maximum value after ~4.5 years of fuel burnup in this test case. The detailed isotopic vectors of the actinide fuels at various fuel burnup steps are plotted in Figure 10, showing consumption of the fissile isotope Pu-239 and the transmutation of the fertile Np-237 and Am-241 isotopes. As shown in Figure 9, the neutron multiplication factor of the fission blanket gradually increases during the time period when the Am-242m concentration increases. It reaches its maximum value of ~0.982 at about 4.5 years in this test case, and then decreases as the blanket fuel is burned.

For obvious safety reasons, fission blanket reactivity should not exceed the specified value at startup. The test case suggests that the increased reactivity could be compensated for by continuous feeding of neutron absorbers into the blanket or by removing actinide fuels from the system. The test case has a very low fission power in the first 4 years of operation when the k_{eff} is low. The system thermal power is ~558 MW at t = 0 when k_{eff} = 0.90. In order to design a more efficient system, the fission blanket should start with high neutron multiplication factors and should then be continuously monitored and adjusted to maintain the same neutron multiplication value.

4.3 Burnup Simulations: Cases I-III

To study fuel burnup in the ADS systems, a Monte Carlo simulation was first performed to simulate the spallation source neutrons generated in the LBE target, utilizing the surface source function in MCNPX [18] without the impact of the fission blanket. In the Monte Carlo model, all zones outside the LBE target except the target assembly are void. Neutron leakage from the LBE target through the target surfaces is recorded, including the characteristic parameters of each neutron. Energy, position, and direction of each neutron are saved in the SSRA source file. The Monte Carlo burnup simulation is then performed with the generated SSRA source file utilizing the MCB5 code. In the fuel burnup simulation, all regions (including the target region) are loaded

with the actual materials, and the external source particles are read from the SSRA file previously generated. Thermal power of the system is fixed at 3 GW, which is used to normalize neutron flux during burnup calculations. The fuel burnup time-step is set to be 90 days per time-step.

During fuel burnup, the neutron multiplication factor will either increase due to the Am-242m buildup or decrease due to the fissile fuel deduction. The continuous or batch feeding or removing techniques of the neutron absorbers or the actinide fuel particles is required in order to control the k_{eff} of the fission blanket at about 0.98 and subsequently, the system fission power.

In this simulation, batch feeding at the end of each time step is utilized to control the k_{eff} of the system. Neutron absorbers are fed into the system when k_{eff} increases. Two major long-lived fission products (LLFPs), Tc-99 and I-129, are added to the fission blankets to decrease the k_{eff} value. Actinide fuel is added into the blanket to compensate for the reactivity loss when k_{eff} decreases. The added fuel composition is the same as the initial actinide fuel particles in the LBE blanket. The approximate amount of feeding materials, neutron absorbers, or actinide fuel materials is calculated so that the k_{eff} of the fission blanket after feeding returns to the initial value of ~0.98. Appendix A shows the mathematical derivation of the simple algorithm for calculating the feeding amount after each time-step, based on the burnup simulation results. The computer codes, which implement the algorithm of Appendix A with MCB5 simulations, are given in Appendixes B and C. Again, Table IV lists the three blanket configurations used in the burnup analyses.

For the three ADS system configurations, the Monte Carlo simulations calculated the k_{eff} at each time step before and after the discrete feeding, and the results are plotted in Figure 11. This figure shows that k_{eff} has been maintained and adjusted to about 0.98 at the end of each time-step after feeding. The amounts of feed materials at each time-step are also shown in Figures 12-14 for the three configurations, respectively. In the configuration with 5% actinide concentration, k_{eff} always decreases within the fuel burnup steps, as shown in Figure 11. For the other two configurations with 7% and 10% actinide concentration in LBE, k_{eff} increases in the first 2 years because there are more MA fuels in the actinide fuel materials and more Am-242m fissile atoms are accumulated, thus compensating for the fissile fuel loss of other isotopes.

Figures 12-14 plot the feeding rates of the LLFPs and the actinides for the three configurations after each time-step, and Figures 15-17 plot the corresponding total amounts of feed materials at the end of each burnup step, respectively. In Figure 12, the annual amount of LLFPs fed into the system is always zero for the configuration with 5% actinide concentration. The annual amount of actinide feed in this configuration increases gradually in the first 6 years of fuel burnup, and then reaches a constant value of about 1.5 ton/year. For the configurations with 7% or 10% actinide concentrations, Figures 13 and 14 show the annual amounts of LLFPs fed into the system for the first two burnup years to compensate for the positive reactivity increases, as shown in Figure 11. Then the actinides are fed to compensate for the reactivity loss due to

burnup. The annual amount of actinides fed into the system gradually increases and saturates at a level of about 1.5 tons/year after 8 to 10 years of burnup. After 10 years of burnup, the total weights of the LLFPs added for the three configurations are 0, 1.18, and 2.15 tons for the configurations with 5, 7, and 10% actinide concentration in the LBE, respectively. The corresponding total actinide amounts are 11.7, 9.35, and 9.03 tons, respectively.

The annual transmutation rates of the total actinides and the MAs are shown in Figure 18 for the three configurations. The transmutation rate of the total actinide fuels is 1.2 tons for the three configurations, because thermal power in the three configurations is fixed at a constant 3 GW_{th}. The ADS systems are very efficient in transmuting MA fuel in the first few years of burnup. For all three configurations, the transmutation rate peaks after about two burnup years and then decreases gradually. The annual transmutation rate of the plutonium increases as the MA transmutation rate decreases. However, at the beginning, plutonium concentration increases because of the production of Pu-238 from the MAs. The transmutation rates of the MAs and the plutonium saturate after about 6 to 10 years of fuel burnup for the three configurations. The asymptotic annual transmutation rates for the MAs and plutonium fuels are calculated to be 0.83 and 0.36 ton/y for the configuration with 5% actinides. Corresponding values for the 7% and 10% actinides are 0.94 and 0.25 ton/y, and 1.02 and 0.17 ton/y, respectively.

The consumed or produced amount of each isotope as a function of burn time for 10 years is shown in Figures 19-21. Table V gives the consumed or produced amount after 10 burnup years. For the three configurations, 11.9 tons of actinides are consumed after 10 years. The system with lower plutonium concentration consumes more MAs fuel and less plutonium fuel. For the configuration with 5% actinides, 6.61 tons of Am-241 and 3.53 tons of Np-237 are consumed. The corresponding values are 7.87 tons of Am-241 and 4.18 tons of Np-237 fuel for the configuration with 7% actinides, and 8.27 tons of Am-241 and 4.42 tons of Np-237 for the configuration with 10% actinides. The weight of Pu-239 fuel consumed by each configuration is 3.55, 2.63, and 1.67 tons, respectively. In addition, after 10 years of operation, 1.66, 2.25, and 2.13 tons of Pu-238; and 0.39, 0.51, and 0.50 tons of Pu-242 are produced for the three configurations, respectively. The corresponding amounts of Cm-244 accumulated are 0.33, 0.36, and 0.32 tons, respectively.

The fuel composition vectors in the LBE as a function of burn time for the three configurations are shown in Figures 22-24. During the first few years of burnup, the fuel vector has a high concentration of Np-237 and Am-241 isotopes. For instance, the configuration with 7% actinides at startup has ~43.4% of Am-241, 24.3% of Np-237, and 17% of Pu-239. After 4 years of burnup, the fuel vector has 22.2% of Am-241, 14.8% of Np-237, and 10.3% of Pu-239. The fraction of Pu-238 increases rapidly, reaching its maximum value of 23.8% after about 6 years of burnup and then slowly decreasing. The Pu-240, Pu-242, and Cm-244 fractions slowly increase with the burnup. Similarly, for the configurations with 5% or 10% actinides, the fractions of Am-241 and Np-237 decrease very rapidly in the first few years of burnup, this in turn increases the Pu-238 fraction. Then after 4 to 6 years of fuel burnup, the Pu-238 fraction decreases due to

burnup and the fractions of other isotopes such as Pu-240, Pu-242, and Cm-244 slowly increase.

The annual amounts consumed per actinide isotope are shown in Figures 25-27 for the 10 burnup years. The results verify that annual consumption of Np-237 and Am-241 decreases very rapidly in the first 6 years of fuel burnup to reach their asymptotic values. Pu-238 concentration increases in the first 4 years. Concentrations of the short half-lived isotopes Am-242m and Cm-242 increase in the first 2 years and then saturate at very low concentrations.

The feeding rates shown in Figures 12-14 and the annual transmutation rates shown in Figure 18 reach asymptotic values after 6 to 10 burnup years, although compositions of the actinide vectors vary slightly during the 10 burnup years, as shown in Figures 22-24. The concentration changes of the major fuel isotopes in the actinide vector, i.e., Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-243, Cm-244, and Cm-245, are very low, and a quasi-equilibrium state is reached after 10 burnup years. In these simulations, actinides are added and the LBE is not processed for removal of the fission products. The only exception is removal of the fission noble gases, i.e., Kr and Xe that leak out of the LBE and are removed from the simulations at the end of each time-step. Because many of the fission products are neutron absorbers, more actinides are fed in these simulations to counteract their effects. The actinide inventories are shown in Figure 28 for the three configurations. These inventories decrease in the first 6 burnup years and then gradually increase. Extra actinides are used to obtain k_{eff} 0.98 because of accumulation of the fission products that act as neutron absorbers. As shown in Table V, the actinide feed is 1.5 tons/year, which is 0.3 ton/year greater than the consumption rate. As a result, the fuel inventory is continuously increasing, as shown in Figure 28. The fission products removal procedure is being studied and will be included in future studies.

In these simulations, the LLFPs are tracked to determine their transmutation rates. Table VI shows the total weights of the LLFP feed at the beginning of the second and third configurations, together with the produced weight from fission or transmutation in the system after 10 burnup years. The transmuted LLFPs amounts are shown in Figures 29-31 for the three configurations. For the configuration with 7% actinides, 0.55 ton of Tc-99 and 0.079 ton of I-129 are transmuted during the 10 burnup years due to their high concentrations relative to the other LLFPs in the LBE. The transmutation rates $<\sigma_\gamma,\phi>$ of each of LLFPs in the three configurations are listed in Table VII. The effective half-lives of the LLFPs in the three configurations range from 6 to 70 years. Therefore, the ADS system is very effective in transmuting the LLFPs, especially Tc-99, which is a dominant LLFP.

5 Summary

In this report, three accelerator-driven subcritical (ADS) system configurations have been proposed for transmuting the 115 metric tons of minor actinides (MAs) in the

70,000 metric tons of the discharged spent nuclear fuel (SNF) planned as the limit in the Yucca Mountain nuclear waste repository. Each configuration has a cylindrical neutron source region at the center, a cylindrical fission blanket outside the source region, and a cylindrical graphite reflector outside the fission blanket. The external neutron source is a spallation source using a 1 GeV proton beam with 25 MW of beam power striking the lead-bismuth eutectic (LBE), or liquid lead, target. The actinide fuel materials are dissolved, mixed, or suspended in the liquid fuel carrier. Therefore, fresh fuel can be fed into the fission blanket to adjust its reactivity and to control system power during operation. A mobile fuel concept with oxide fuel particles suspended in the LBE has been adopted to form the fission blanket.

Steady-state Monte Carlo simulations using the MCNPX code have been performed to determine the overall parameters. Source region geometry is determined so as to satisfy the energy deposition limit imposed on the target window and the corrosion limit of the structure materials to accommodate the required 25 MW proton beam power. The neutron multiplication factor k_{eff} of the fission blanket is determined to be approximately 0.98 so that the 25 MW proton beam can produce 3 GW_{th} of fission power. Thickness of the graphite reflector outside the fission blanket is set at 250 cm to improve the k_{eff} of the fission blanket. Fuel composition is based on the LWR discharged fuels considered for the Yucca Mountain analysis. Because the main goal of the ADS system is to transmute MA fuel, plutonium consumption is minimized. Plutonium concentration is adjusted to achieve 0.98 k_{eff}, and the MA inventory in the fission blanket does not exceed 10 tons.

The results from the Monte Carlo steady state simulations have defined three possible configurations for the fission blanket with 5, 7, and 10% actinides in LBE to have 0.98 k_{eff} and ~10 tons of MA initial inventory. Monte Carlo fuel burnup simulations using the MCB5 code have been performed to analyze the performance of the three configurations. The ENDF/B-VII.0 nuclear data files have been utilized in the burnup calculations, and the Am-241 neutron capture branch ratio to Am-242m has also been updated in the MCB5 code. Fission power was fixed at 3 GW_{th} during the burnup calculations.

According to the MCB5 burnup results, the three configurations consume about 1.2 tons of actinides per year. However, the annual transmutation rate of MAs is slightly higher with more actinides in the LBE. Total MA weights consumed during the first 10 years of operation are 9.85, 11.80, or 12.68 tons for the configurations with 5, 7, or 10% actinides in the LBE, respectively. The corresponding annual MA fuel transmutation rates are 0.83, 094, and 1.02 tons/year for the three configurations, respectively, after reaching equilibrium at 10 burnup years. Therefore, the total MA weights burned by the three configurations are 30.6, 35.3, and 37.2 tons, respectively, assuming that the ADS system can be operated for 35 years. To utilize the 115 tons of MAs from the 70,000 tons of SNF, 3.8, 3.3, or 3.1 ADS systems are required for the three configurations considered in the study, respectively.

References

[1] DOE Office of Civilian Radioactive Waste Management, "Draft Environmental Impact Statement for a Geologic Repository – Appendix A: Inventory and Characteristics of Spent Nuclear Fuel, High-Level Radioactive Waste, and Other Materials," ODE/EIS-0250D, July 1999.

[2] R. N. Hill, "LWR Feed Inventory Specification for ATW System Studies," INTRA-LABORATORY MEMO, June 2000.

[3] DOE Office of Civilian Radioactive Waste Management, "A Roadmap for Developing Accelerator Transmutation of Waste (ATW) Technology – A Report to Congress," DOE/RW-0519, Oct. 1999.

[4] The European Technical Working Group on ADS System, "A European Roadmap for Developing Accelerator Driven Systems (ADS System) for Nuclear Waste Incineration," April 2001.

[5] Nuclear Energy Agency, OECD, "Physics and Safety of Transmutation Systems, A Status Report," ISBN 92-64-01082-3, 2006.

[6] W. Maschek, X. Chen, F. Delage, A. Fernandez-Carretero, D. Haas, C. Matzerath Boccaccini, A. Rineiski, P. Smith, V. Sobolev, R. Thetford, and J. Wallenius, "Accelerator Driven Systems for Transmutation: Fuel Development, Design and Safety," *Prog. Nucl. Eng.*, **50**, 333-340, 2008.

[7] K, TSUJIMOTO, T. SASA, K. NISHIHARA, H. OIGAWA, and H. TAKANO, "Neutronics Design for Lead-Bismuth Cooled Accelerator-Driven System for Transmutation of Minor Actinide," *J. Nucl. Sci. Tech.*, **41**, 21-26, 2004.

[8] H. T. HAHN, "Uranium Oxide – Liquid Metal Slurries," *Industrial and Engineering Chemistry*, **51**, 2, 197-199, 1959.

[9] B. Becker, M. Fratoni, and E. Greenspan, "Feasibility of a Critical Molten Salt Reactor for Waste Transmutation," *Prog. Nucl. Eng.*, **50**, 236-241, 2008.

[10] Y. Gohar, P. J. Finck, L. Krajtl, J. E. Herceg, W. D. Pointer, J. Saiveau, T. Sofu, A. L. Hanson, M. Todosow, M. Koploy, and P. Jijatovic, "Lead-Bismuth Target Design for the Subcritical Multiplier (SCM) of the Accelerator Driven Test Facility (ADTF)," ANL/TD/02-01, Argonne National Laboratory, Jan. 2002.

[11] S. Andriamonje, et al., "Experimental determination of the energy generated in nuclear cascades by a high energy beam," *Phy. Letter B*, **348**, 697-709, 1995.

[12] OECD/NEA Nuclear Science Committee, Working Party on Scientific Issues of the Fuel Cycle, Working Group on Lead-bismuth Eutectic, “Handbook on Lead-bismuth Eutectic Alloy and Lead Properties, Materials Compatibility, Thermal-hydraulics and Technologies,” ISBN 978-92-64-99002-9, 2007 Edition.

[13] Alloy Phase Diagram Center, http://www1.asminternational.org/asmenterprise/apd.

[14] L. Golyand, E. Shwageraus, and Y. Ron, “Effect of $^{95}{}_{241}$Am(n,g) Reaction Branching Ratio on Fuel Cycle and Reactor Design Characteristics,” *Nucl. Sci. Eng.*,**161**,289-302, 2009.

[15] M. B. Chadwick, et al., “ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology,” *Nuclear Data Sheets*, **107**, 2931-3060, 2006.

[16] J. Cetnar, W. Gudowski, and J. Wallenius, “User Manual for Monte-Carlo Continuous Energy Burnup (MCB) Code – Version 1C.”

[17] F. M. Mann and R. E. Schenter, “Calculated Neutron Capture Cross Sections to the Americium Ground and Isomeric States,” *Nucl. Sci. Eng.*, **63**, 242-249, 1977.

[18] D. B. Pelowitz, “MCNPX User’s Manual, Version 2.6.0,” LA-CP-07-1473, April 2008.

Table I. Main parameters of LBE target designs.

Parameters	Old ANL Design	New Design
Proton Beam Energy (MeV)	600	1000
Proton Beam Power (MW)	5	25
Proton Beam Radius (with halo current) (cm)	10.0	19.5
LBE Coolant Outlet Flow Channel Radius (cm)	13.2	27.8
LBE Coolant Inlet Flow Channel Radius (cm)	16.5	33.8
Steel Outer Wall Radius (cm)	17.0	35.0
Target Length (cm)	35.0	70.0
Target Radius (cm)	16.5	33.8

Table II. Physical properties of ADS system materials.

Parameters	Temp. (K)	Mass density (g/cc)	Compositions and atomic fraction (%)
LBE in target	600	10.3	Pb206 10.93 Pb207 10.01 Pb208 23.76 Pb209 55.30
Steel	600	7.87	Fe54 5.85 Fe56 91.75 Fe57 2.12 Fe58 0.28
LBE in blanket	900	9.91	Pb206 10.93 Pb207 10.01 Pb208 23.76 Pb209 55.30
Actinide fuel in blanket	900	---	U235 4.08E-3 U236 2.03E-3 U238 0.481 Pu238 1.28 Pu239 53.31 Pu240 21.49 Pu241 3.76 Pu242 4.64 Np237 5.08 Am241 8.91 Am242m 1.38E-2 Am243 0.91 Cm243 1.97E-3 Cm244 0.10 Cm245 8.80E-3 Cm246 9.74E-4
Graphite	600	1.6	C12 1.0

Table III. Energy multiplication of 25 MW proton beam power with 1 GeV protons from various fission blanket configurations.

K_{eff}	Actinide loading	Plutonium loading	Diameter/ height (m)	Energy multiplication factor	Fission power (GW)
0.97974	5%	40%	2.40	127	3.180
0.97908	5%	35%	3.12	123	3.070
0.97920	5%	30%	5.00	117	2.910
0.98030	7%	35%	2.05	117	2.920
0.98069	7%	30%	2.54	122	3.050
0.97940	7%	25%	3.56	113	2.825

Table IV. Three fission blanket configurations with 0.98 k_{eff} and MA inventory ≤ 10 tons.

K_{eff}	Actinide loading	Plutonium loading	Volume (m^3)	Height/ diameter(m)	MA loading (ton)
0.980	5%	35.7%	20.4	3.0	6.33
0.980	7%	27.2%	20.4	3.0	10.0
0.980	10%	20.0%	13.7	2.64	10.6

Table V. Annual feeding rates, annual transmutation rates at tenth year of fuel burnup, and total transmutation after first ten burnup years for the three fission blanket configurations in Table IV.

Isotope	Feeding rate (ton/y)			Transmutation rate (ton/y)			Total transmutation (ton)		
	Ac 5%	Ac 7%	Ac 10%	Ac 5%	Ac 7%	Ac 10%	Ac 5%	Ac 7%	Ac 10%
U-234	---	---	---	-5.5E-3	-8.0E-3	-7.5E-3	-0.066	-0.096	-0.092
U-235	2.6E-5	1.9E-5	1.4E-5	-1.0E-3	-1.6E-3	-1.5E-3	-0.011	-0.014	-0.013
U-236	1.3E-5	9.6E-6	7.2E-6	-6.9E-4	-8.0E-4	-7.3E-4	-0.004	-0.004	-0.004
U-238	3.1E-3	2.3E-3	1.7E-3	1.6E-3	1.2E-3	8.7E-4	0.015	0.011	0.008
Np-237	3.3E-1	3.6E-1	4.1E-1	2.9E-1	3.3E-1	3.5E-1	3.532	4.182	4.422
Pu-238	8.2E-3	6.1E-3	4.6E-3	-2.3E-2	-5.5E-3	2.9E-3	-1.659	-2.250	-2.128
Pu-239	3.4E-1	2.6E-1	1.9E-1	3.0E-1	2.2E-1	1.4E-1	3.554	2.632	1.673
Pu-240	1.4E-1	1.0E-1	7.7E-2	7.8E-2	4.7E-2	3.2E-2	0.524	0.316	0.222
Pu-241	2.4E-2	1.8E-2	1.4E-2	1.5E-2	9.6E-3	6.3E-3	0.066	0.042	0.033
Pu-242	3.0E-2	2.2E-2	1.7E-2	-8.1E-3	-1.4E-2	-1.2E-2	-0.390	-0.514	-0.498
Am-241	5.9E-1	6.5E-1	7.3E-1	5.2E-1	5.9E-1	6.1E-1	6.607	7.873	8.272
Am-242	---	---	---	1.3E-6	-3.7E-6	3.3E-4	-0.001	-0.001	0.001
Am-242m	9.2E-4	1.0E-3	1.1E-3	-3.1E-3	-3.0E-3	3.7E-3	-0.062	-0.090	-0.058
Am-243	6.1E-2	6.7E-2	7.5E-2	4.1E-2	4.8E-2	5.3E-2	0.413	0.511	0.574
Cm-242	---	---	---	5.1E-4	1.8E-4	2.2E-2	-0.200	-0.223	-0.108
Cm-243	1.3E-4	1.5E-4	1.6E-4	5.5E-4	6.6E-4	5.9E-4	-0.015	-0.015	-0.015
Cm-244	6.8E-3	7.6E-3	8.5E-3	-1.4E-2	-1.5E-2	-1.1E-2	-0.330	-0.355	-0.321
Cm-245	5.9E-4	6.5E-4	7.3E-4	-3.5E-3	-4.1E-3	-3.6E-3	-0.062	-0.066	-0.063
Cm-246	6.5E-5	7.3E-5	8.1E-5	-3.1E-3	-3.2E-3	-3.0E-3	-0.026	-0.024	-0.023
Cm-247	---	---	---	-4.3E-4	-4.2E-4	-3.9E-4	-0.003	-0.003	-0.002
Cm-248	---	---	---	-1.9E-4	-1.4E-4	-1.3E-4	-0.001	-0.001	-0.001
Total_UPu	0.535	0.408	0.30	0.36	0.25	0.16	2.03	0.12	-0.80
Total_MA	0.965	1.092	1.20	0.83	0.94	1.02	9.85	11.80	12.78
Total_Ac	1.5E+0	1.5E+0	1.5E+0	1.2E+0	1.2E+0	1.2E+0	11.88	11.91	11.88

Table VI. Total feed, total production from fission reactions, and total transmutations of LLFPs after first ten burnup years for the three fission blanket configurations in Table IV.

Isotope	Feed (ton)			Production from fission (ton)			Total transmutation (ton)		
	Ac 5%	Ac 7%	Ac 10%	Ac 5%	Ac 7%	Ac 10%	Ac 5%	Ac 7%	Ac 10%
Se-79	---	---	---	0.0012	0.0013	0.0014	0.0002	0.0002	0.0002
Zr-79	---	---	---	0.191	0.193	0.192	0.0083	0.0062	0.0057
Tc-99	---	0.96	1.75	0.295	0.298	0.297	0.081	0.550	0.945
Pd-107	---	---	---	0.132	0.133	0.135	0.039	0.036	0.038
I-129	---	0.22	0.40	0.107	0.111	0.114	0.015	0.079	0.136
Cs-135	---	---	---	0.334	0.369	0.370	0.020	0.023	0.023
Total LLFP	---	1.18	2.15	1.06	1.11	1.11	0.164	0.694	1.15

Table VII. Transmutation rates and effective half-lives of LLFPs after first ten burnup years for the three fission blanket configurations in Table IV.

LLFP	Ac 5%		Ac 7%		Ac 10%	
	$<\sigma_\gamma,\phi>$ (s^{-1})	$T_{1/2}$(y)	$<\sigma_\gamma,\phi>$ (s^{-1})	$T_{1/2}$(y)	$<\sigma_\gamma,\phi>$ (s^{-1})	$T_{1/2}$(y)
Se-79	1.46E-09	15.0	1.21E-09	18.2	1.22E-09	18.0
Zr-93	4.03E-10	54.6	3.29E-10	66.8	3.25E-10	67.7
Tc-99	2.80E-09	7.8	2.33E-09	9.4	2.38E-09	9.2
Pd-107	4.06E-09	5.4	3.45E-09	6.4	3.59E-09	6.1
I-129	1.31E-09	16.8	1.11E-09	19.9	1.15E-09	19.2
Cs-135	7.96E-10	27.6	6.57E-10	33.5	6.60E-10	33.3

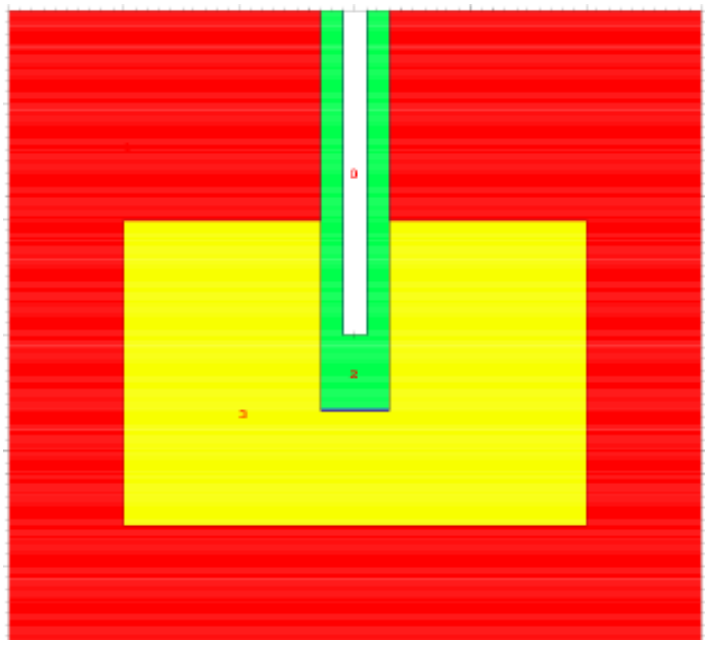


Figure 1. ADS system schematic representation (White: proton beam current channel; Green: LBE target/coolant; Blue: HT-9 wall; Yellow: LBE fuel blanket; Red: graphite).

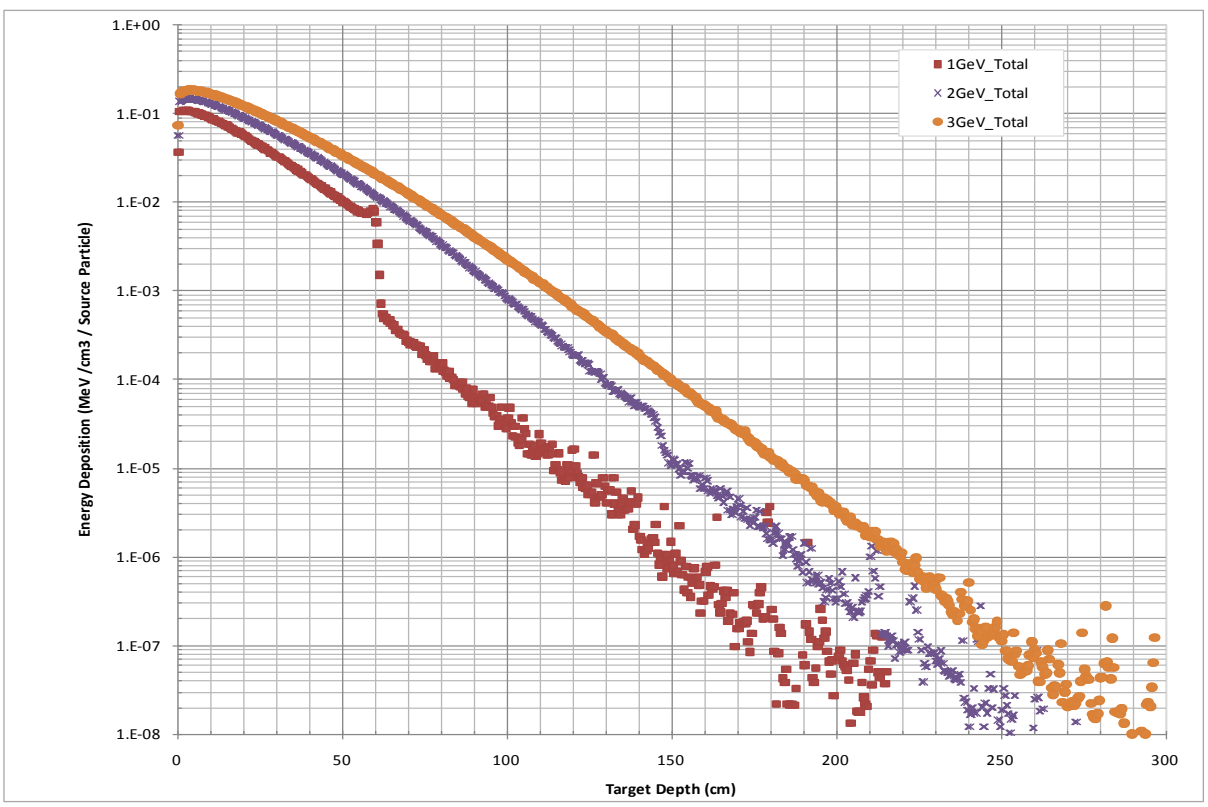


Figure 2. LBE total energy deposition as function of target length for various proton energies.

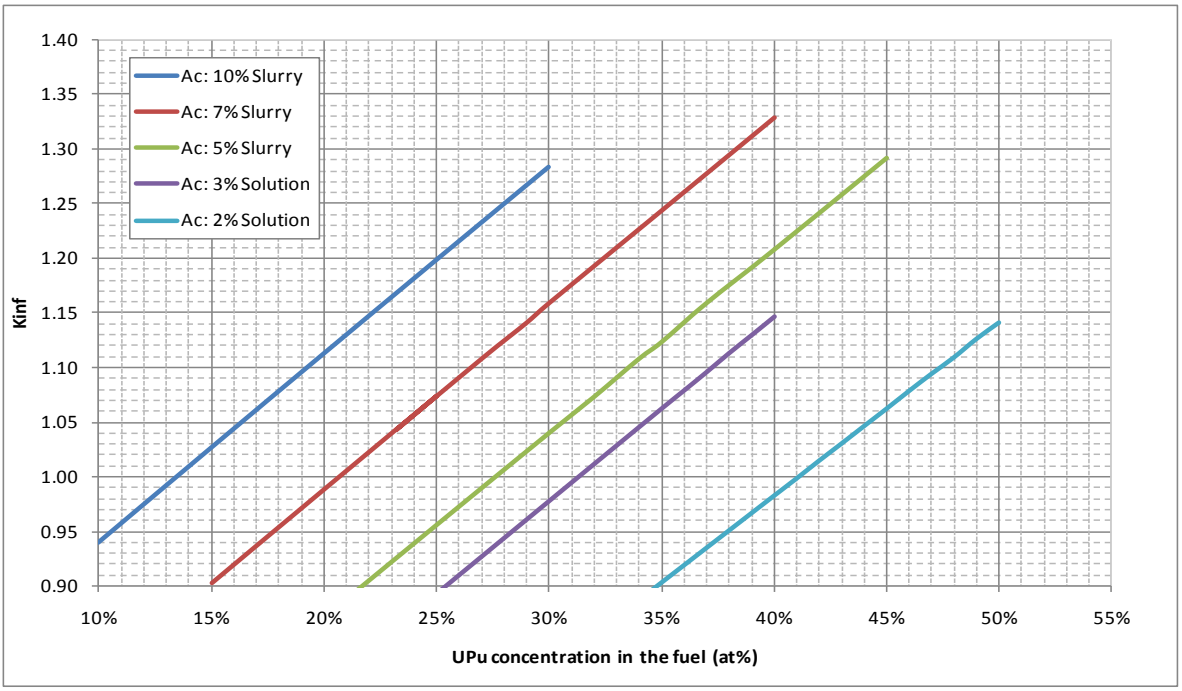


Figure 3 Fission blanket infinite neutron multiplication as a function U-Pu concentration in actinide mixture for various actinide concentrations in LBE fuel carrier of blanket.

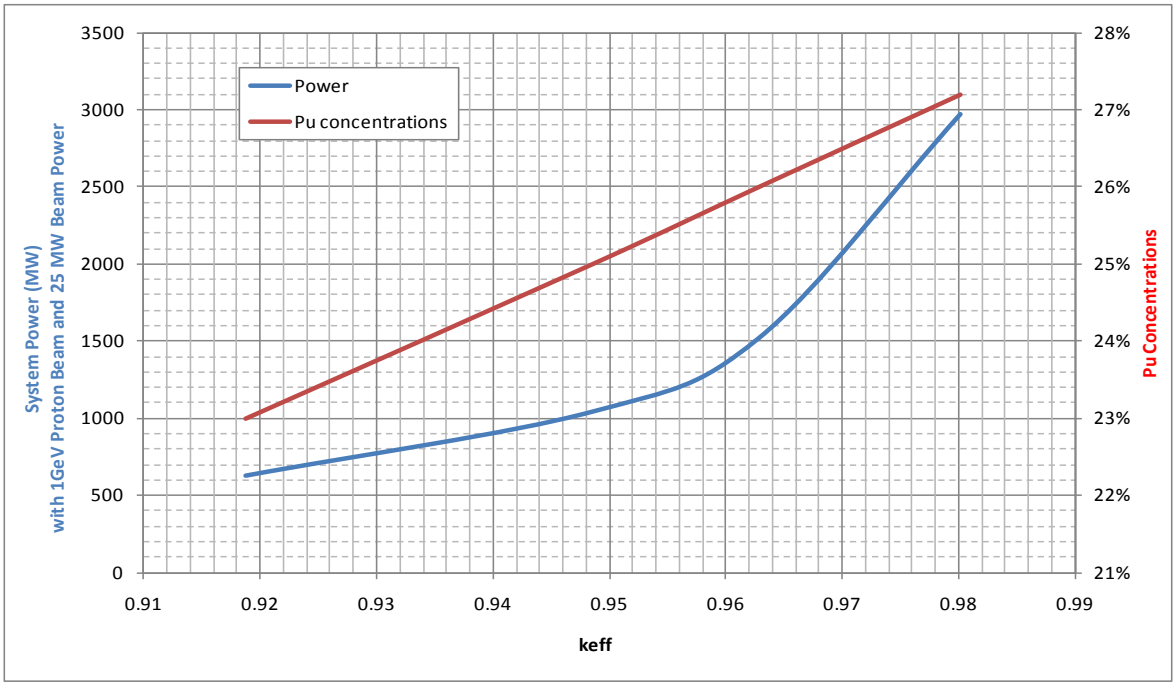


Figure 4 Fission blanket effective neutron multiplication with 7% actinides in LBE fuel carrier as a function of plutonium concentration in actinide mixture and corresponding total power in ADS system obtained by 1GeV proton beam with 25 MW beam power at each k_{eff} value.

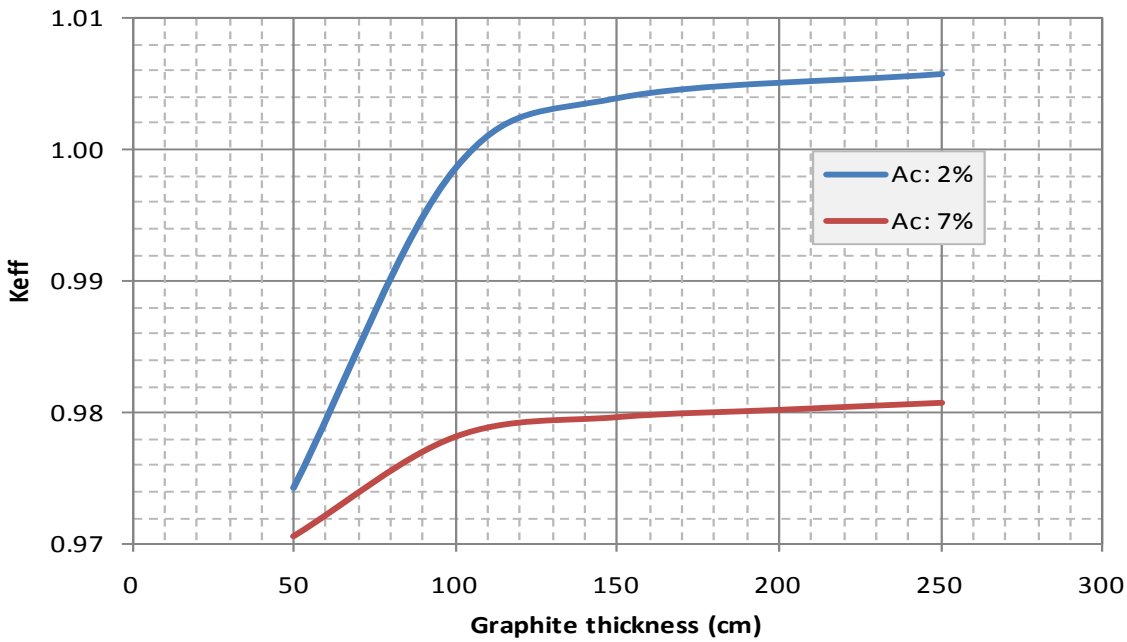


Figure 5 Fission blanket effective neutron multiplication with 2% actinides consisting of 50% plutonium and 7% actinides consisting of 27.2% plutonium in LBE fuel carrier as a function of graphite reflector thickness.

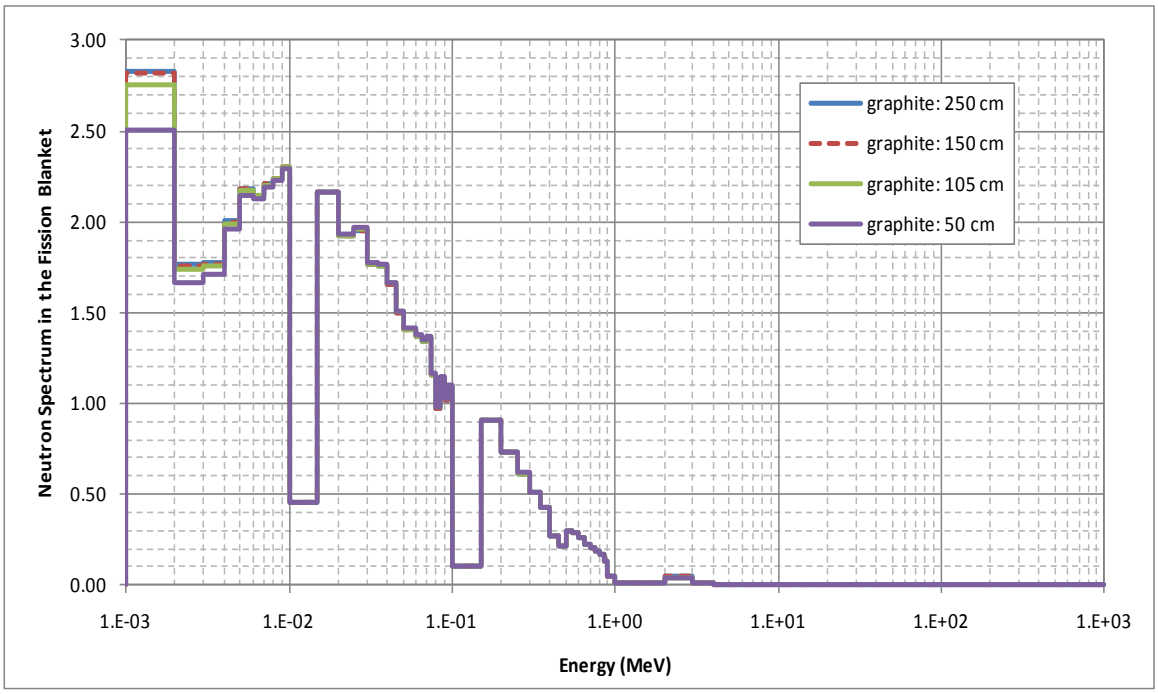


Figure 6 Fission blanket neutron spectra with 7% actinides consisting of 27.2% plutonium fraction in LBE fuel carrier for various graphite reflector thicknesses.

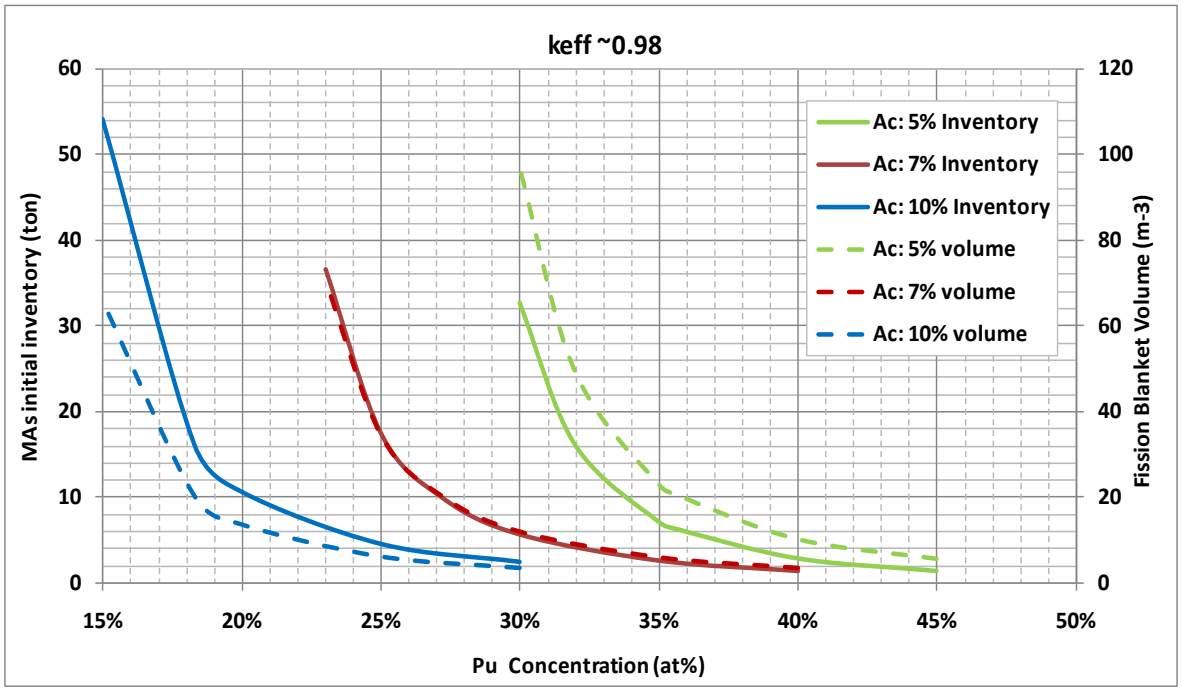


Figure 7 Minor actinide inventories in fission blankets with 0.98 effective neutron multiplication factor and their volumes as a function of plutonium concentration in actinide mixture for three blanket configurations with 5, 7, and 10% actinide concentration in LBE fuel.

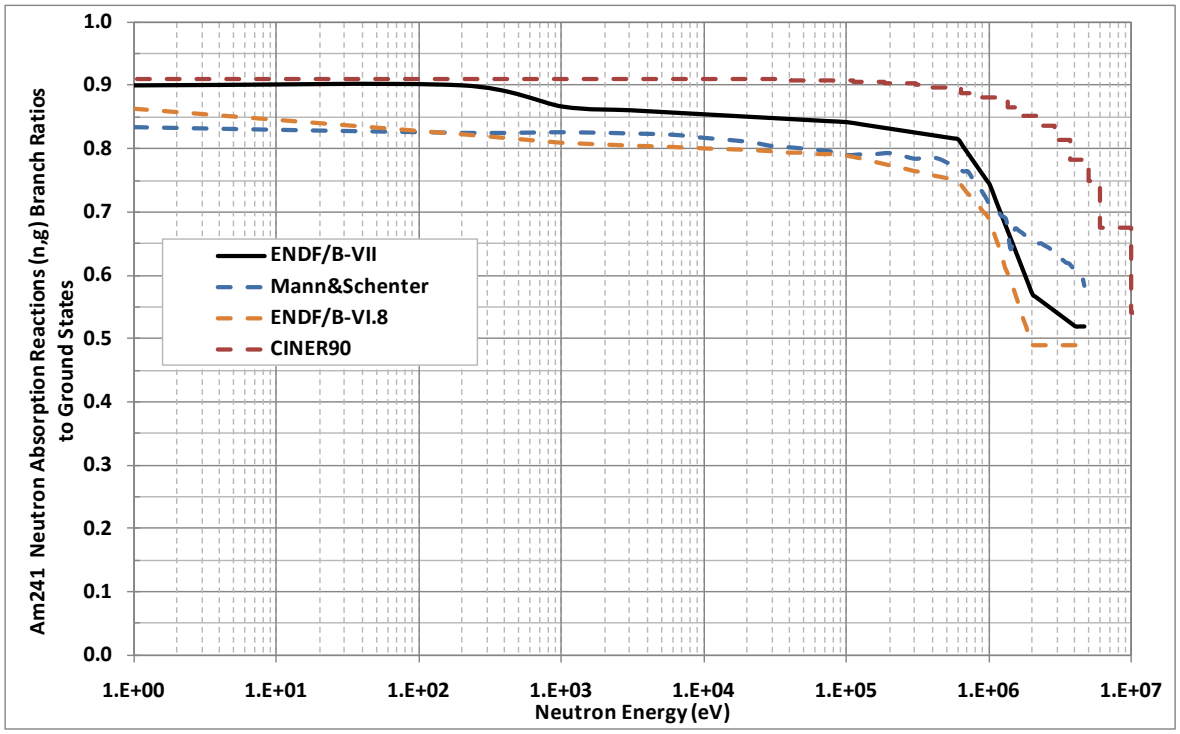


Figure 8 Am-241(n,g)Am-242g branching ratios from Mann & Schneter calculation, ENDF/B-VI.8, –VII.0 nuclear data files, and CINDER90 library.

Figure 9 Effective neutron multiplication factor and Am-242m concentration in test blanket for first 5 burnup years driven by 25 MW beam power using 1 GeV protons.

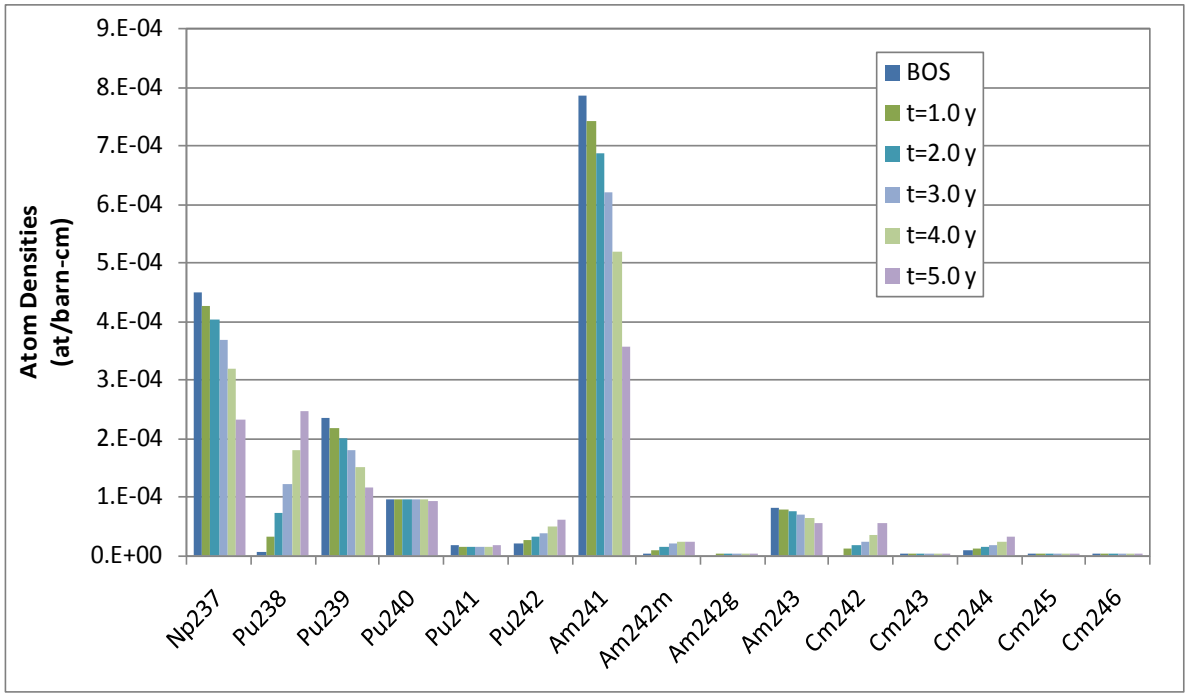


Figure 10 Actinide fuel compositions in test blanket for first 5 burnup years driven by 25 MW beam power using 1 GeV protons.

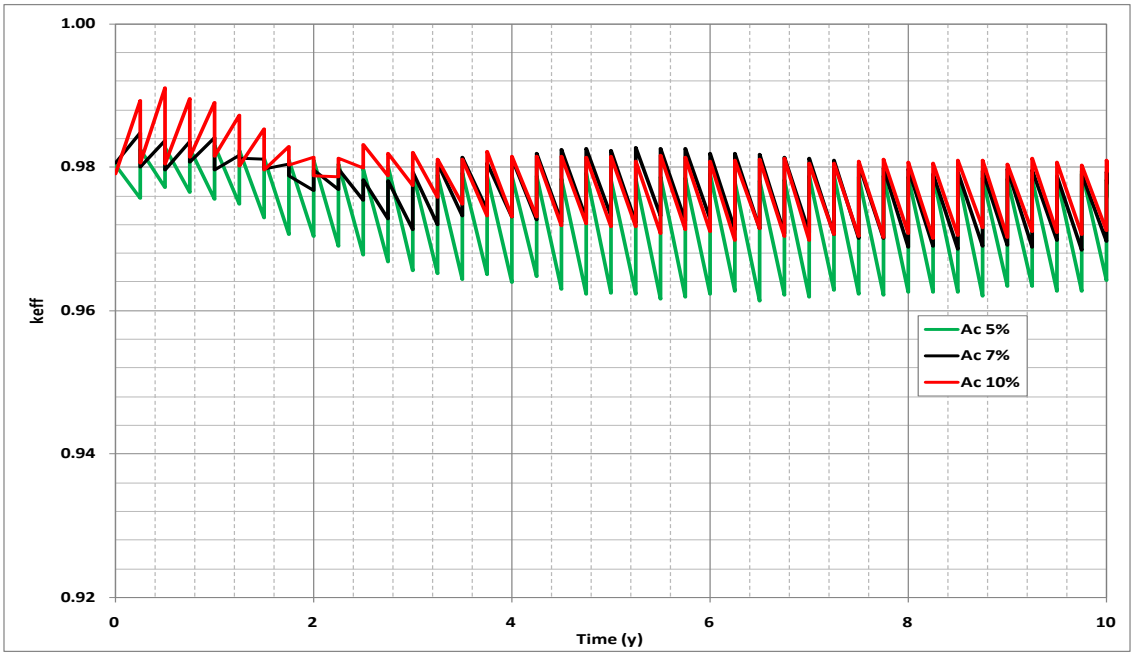


Figure 11 Effective neutron multiplication value before and after each fuel burnup time step for the three fission blanket configurations of Table IV.

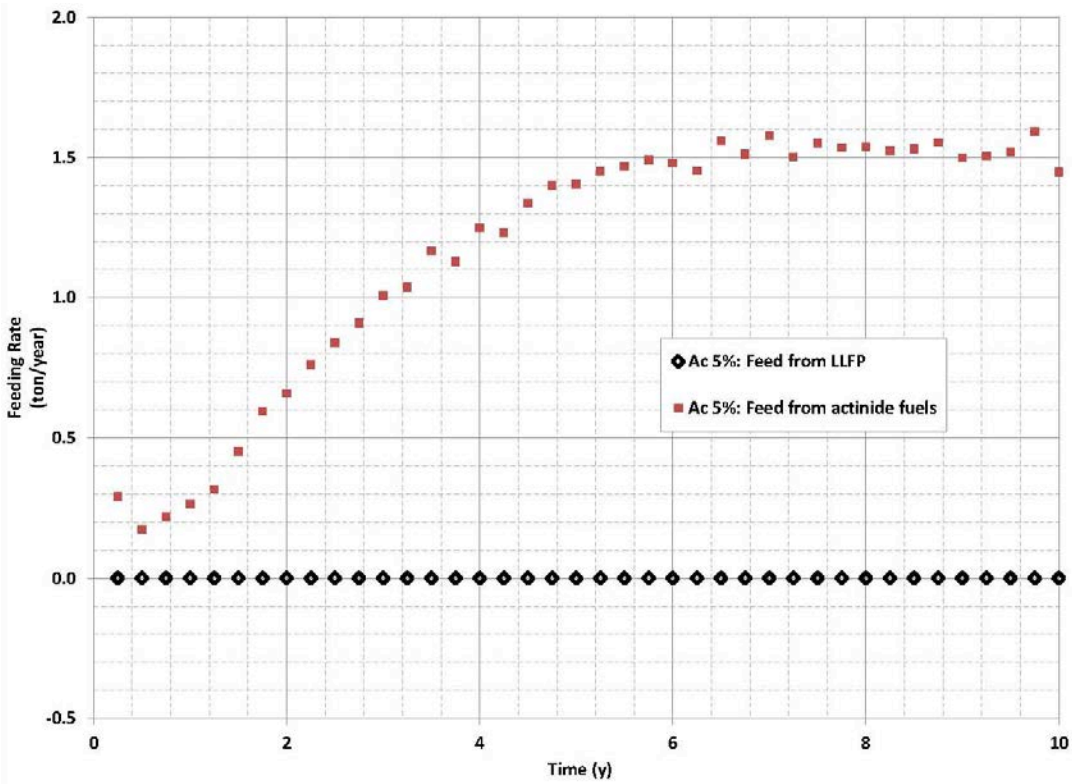


Figure 12 Actinides and LLFPs annual feeding rates at end of each burnup step for blanket configuration with 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides.

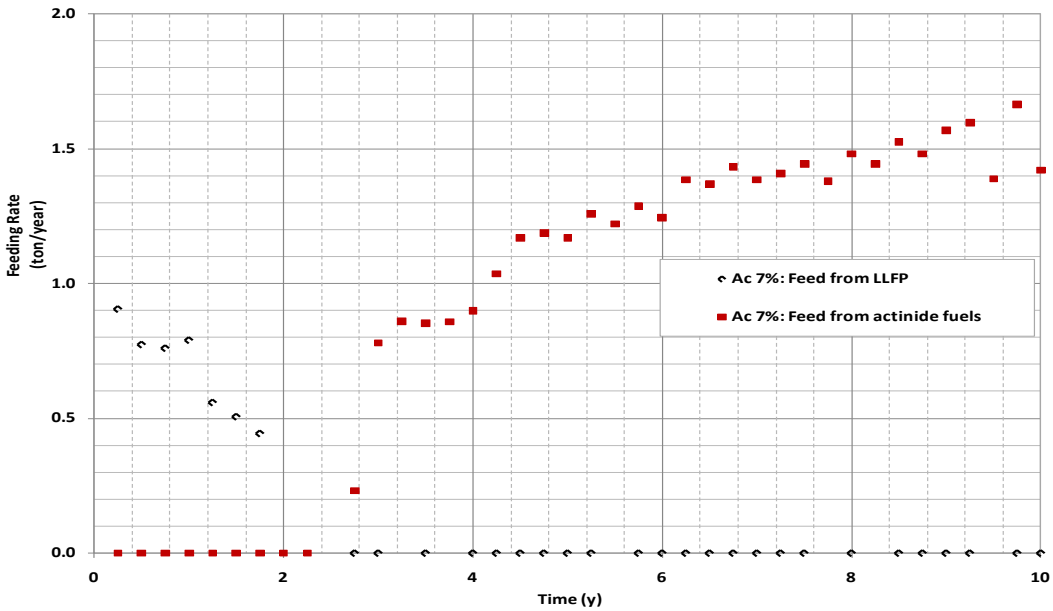


Figure 13 Actinides and LLFPs annual feeding rates at end of each burnup step for the blanket configuration with 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides.

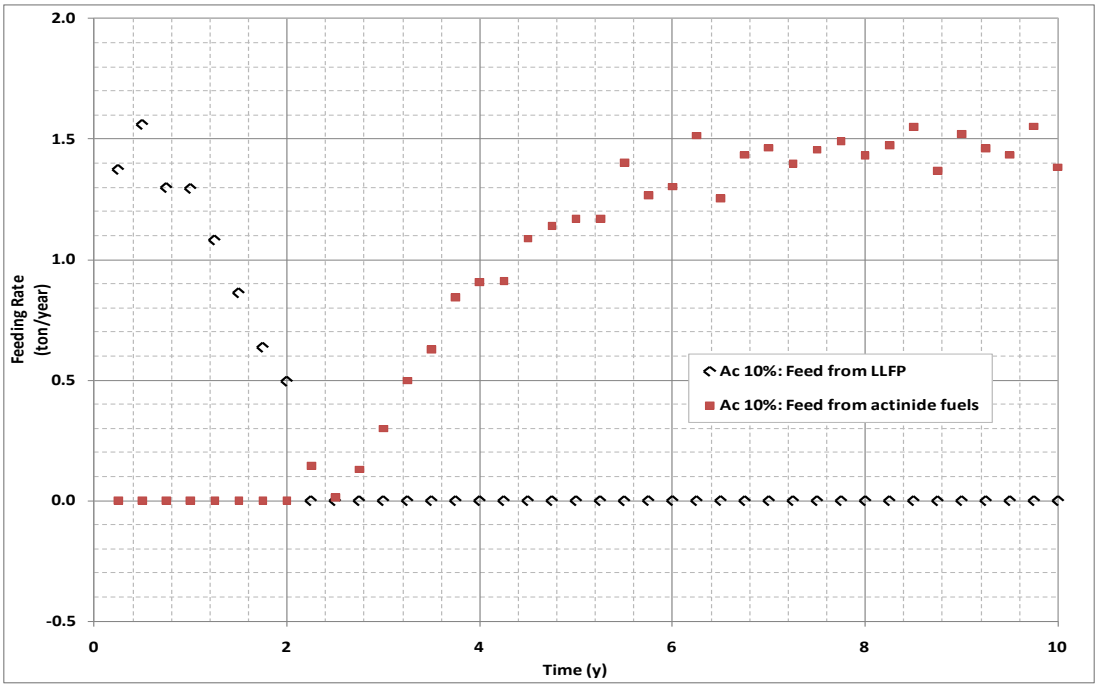


Figure 14 Actinides and LLFPs annual feeding rates at end of each burnup step for the blanket configuration with 10% actinide concentration in LBE and 20% plutonium concentration in actinides.

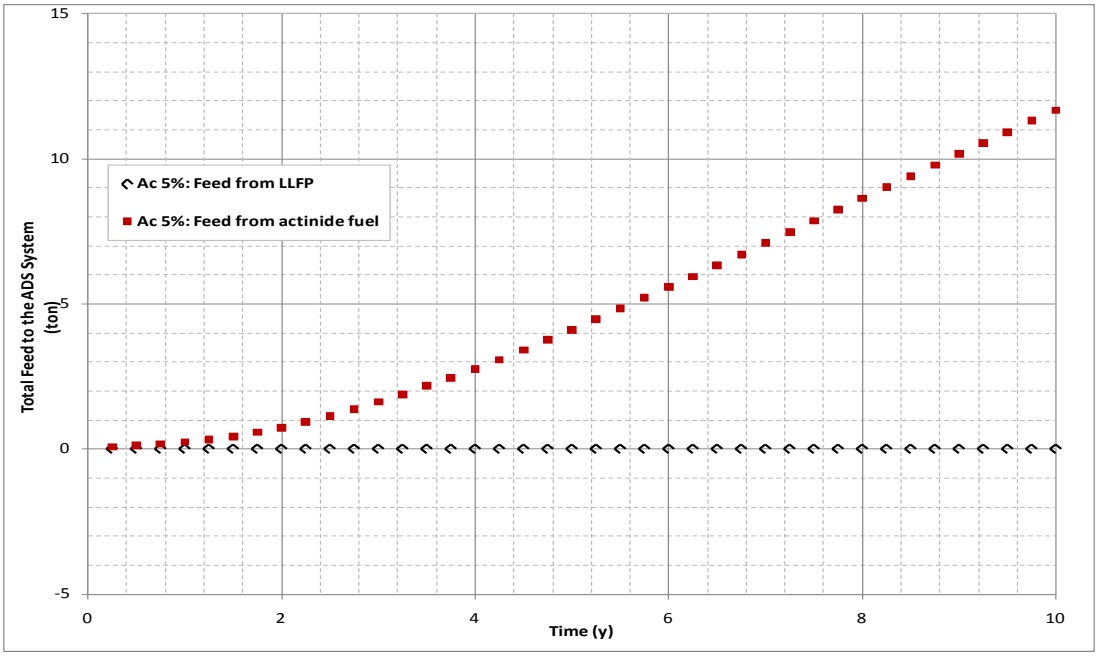


Figure 15 Total actinides and LLFPs feed at end of each burnup step for blanket configuration with 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides.

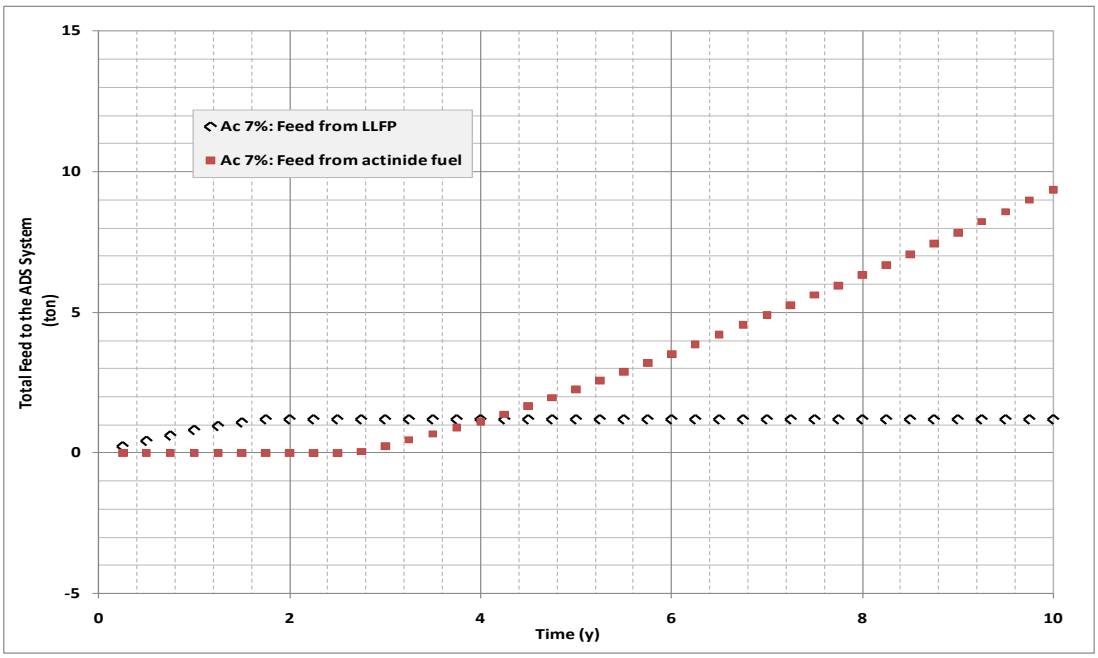


Figure 16 Total actinides and LLFPs products feed at end of each burnup step for blanket configuration with 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides.

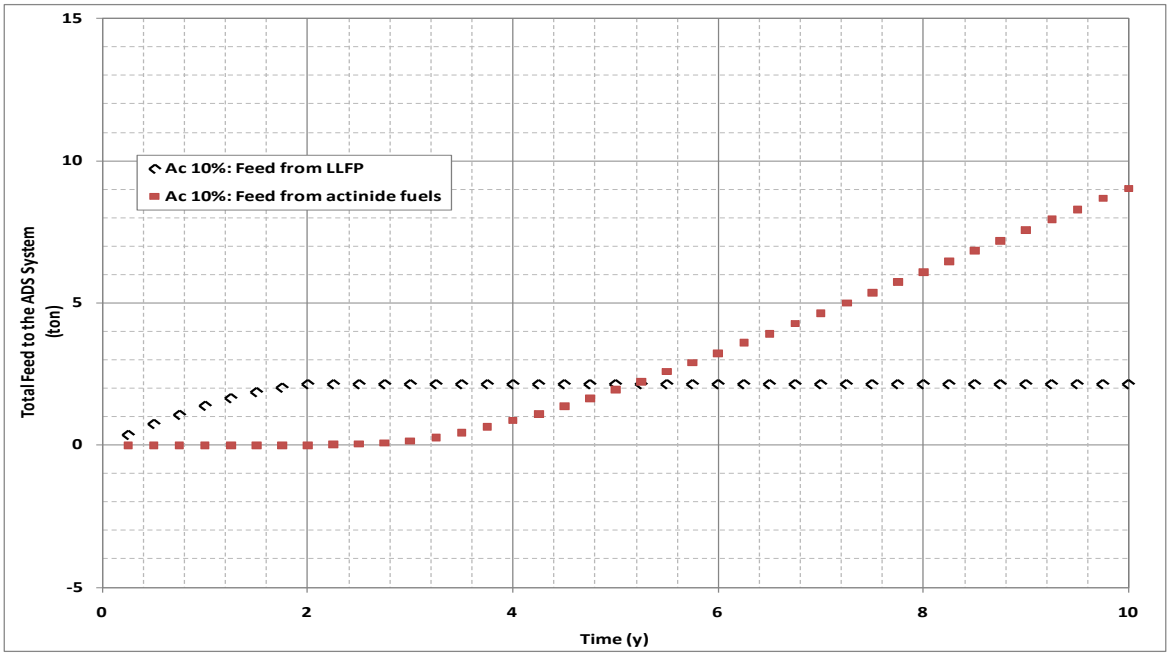


Figure 17 Total actinides and LLFPs feed at end of each burnup step for blanket configuration with 10% actinide concentration in LBE and 20% plutonium concentration in actinides.

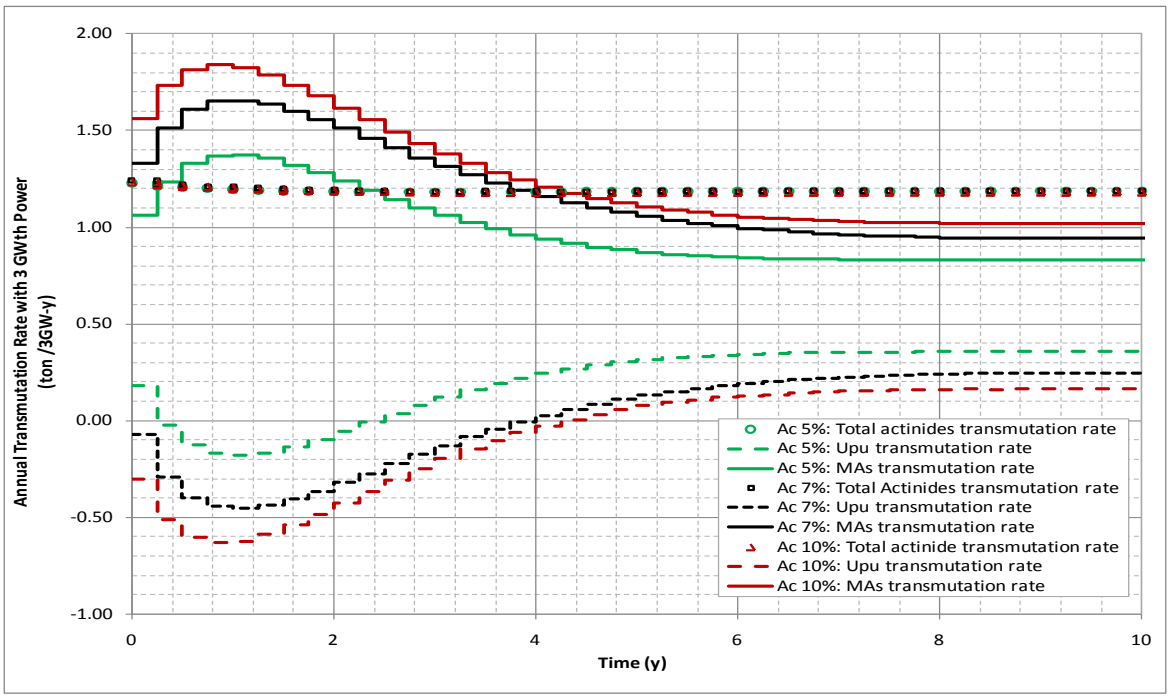


Figure 18 Actinides, U-Pu, and MAs transmutation rates for three blanket configurations of Table IV.

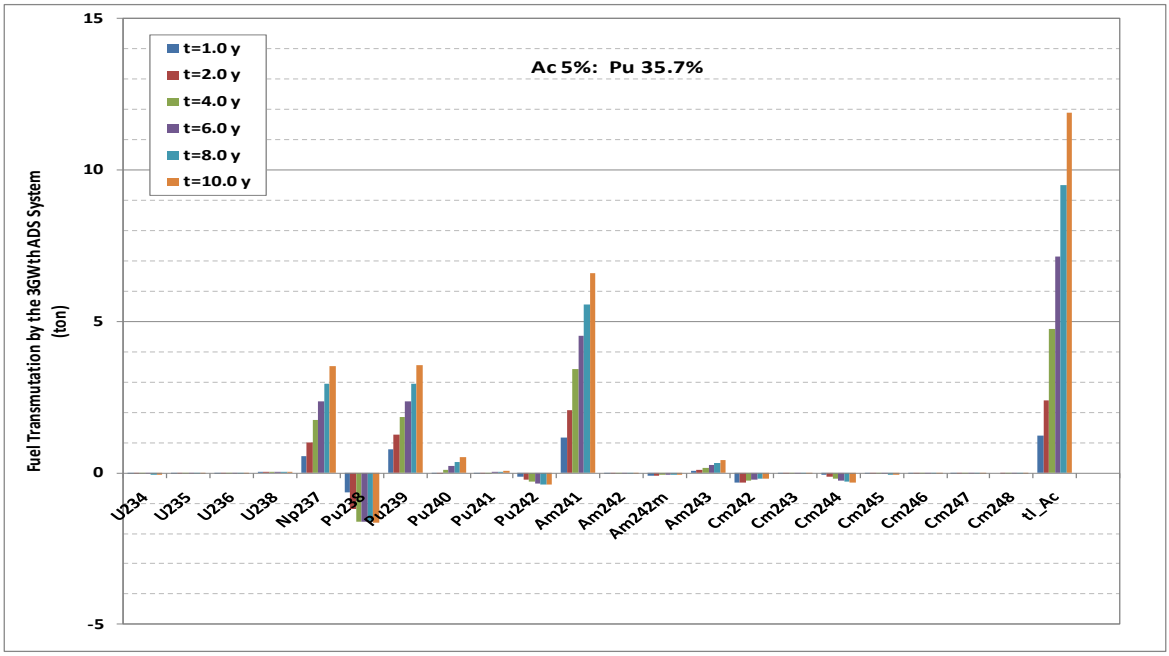


Figure 19 Consumption of actinide isotopes during first 10 burnup years for blanket configuration with 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides.

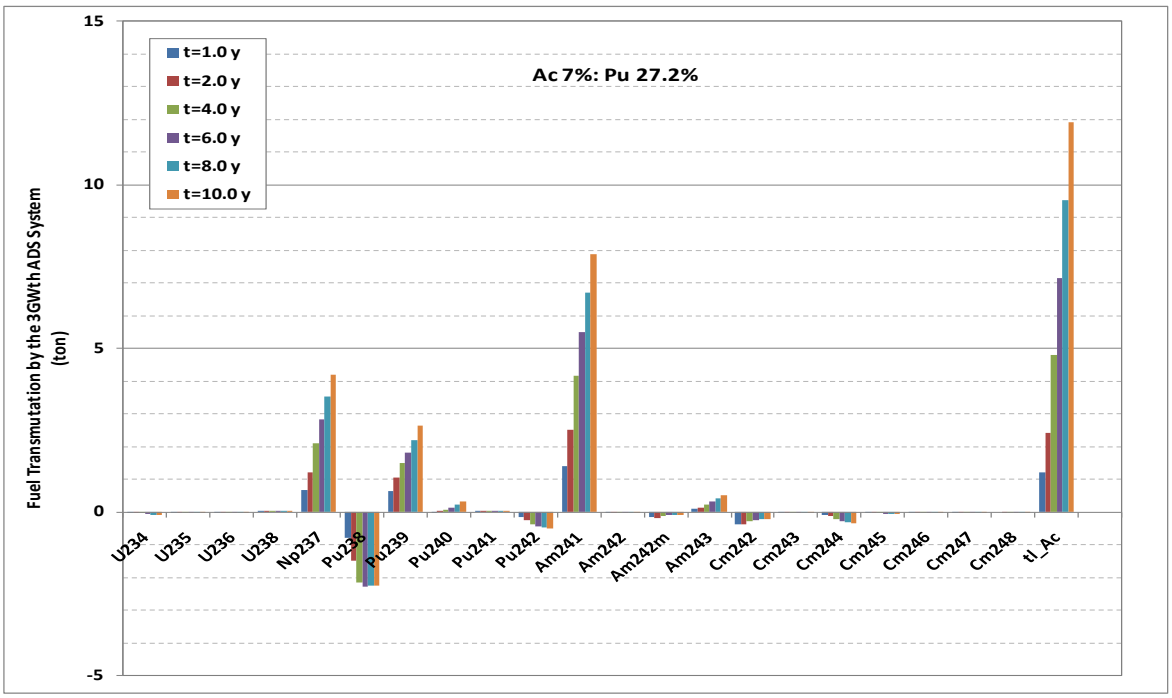


Figure 20 Consumption of actinide isotopes during first 10 burnup years for blanket configuration with 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides.

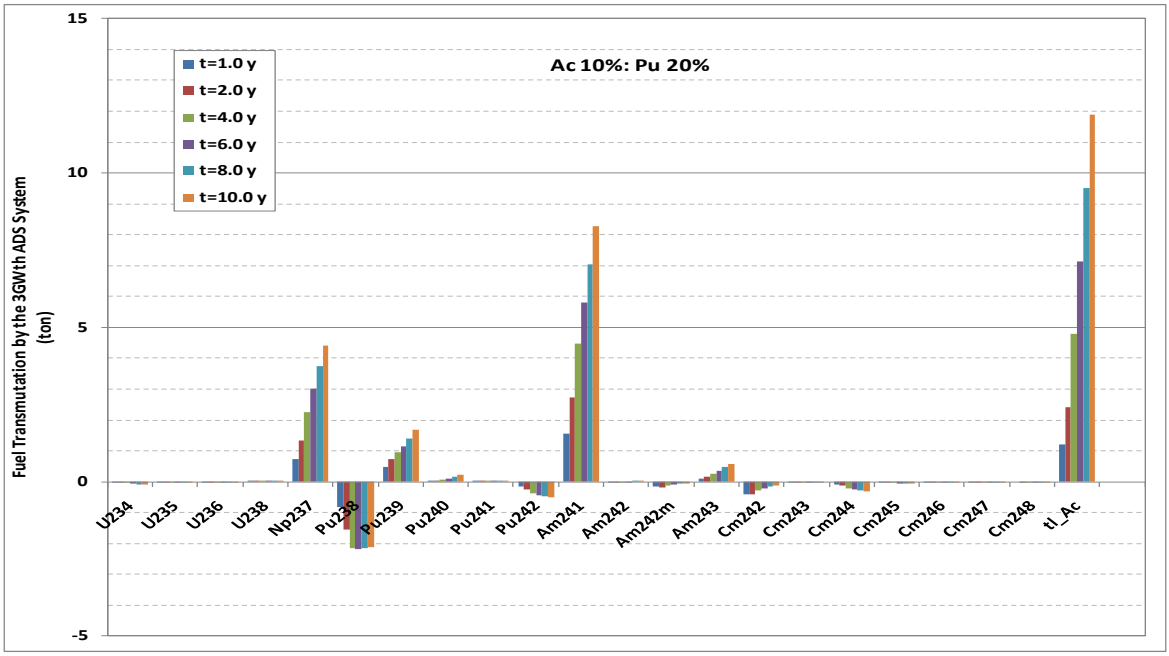


Figure 21 Consumption of actinide isotopes during first 10 burnup years for blanket configuration with 10% actinide concentration in LBE and 20% plutonium concentration in actinides.

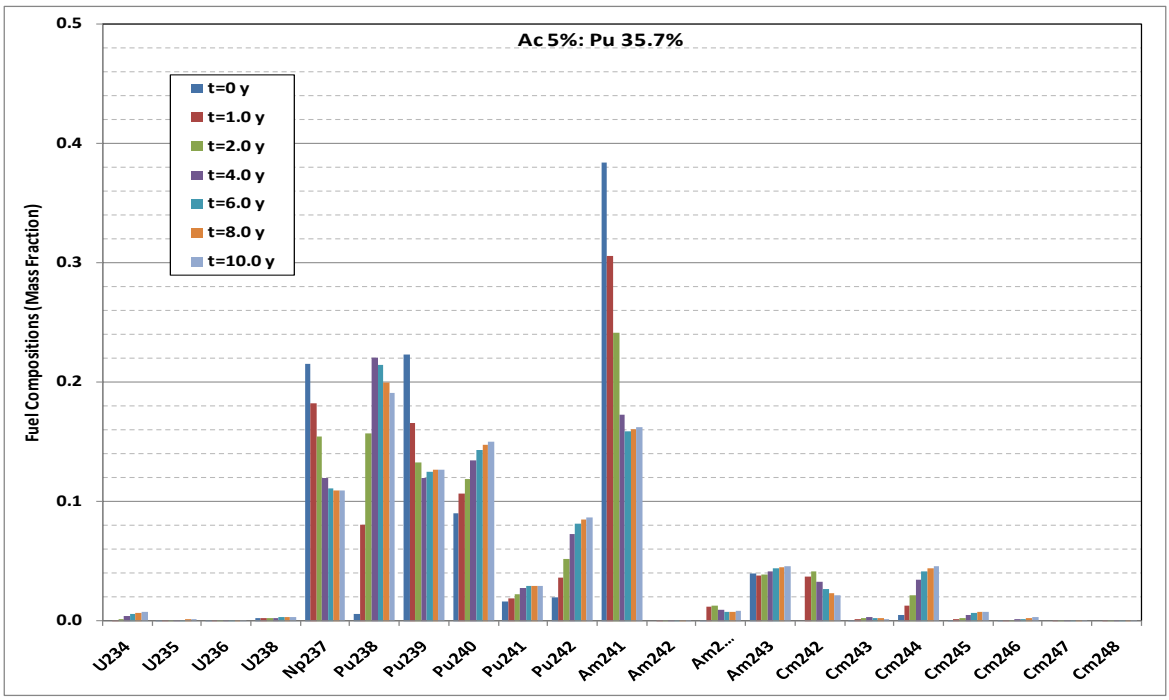


Figure 22 Actinide isotopic compositions during first 10 burnup years for blanket configuration 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides.

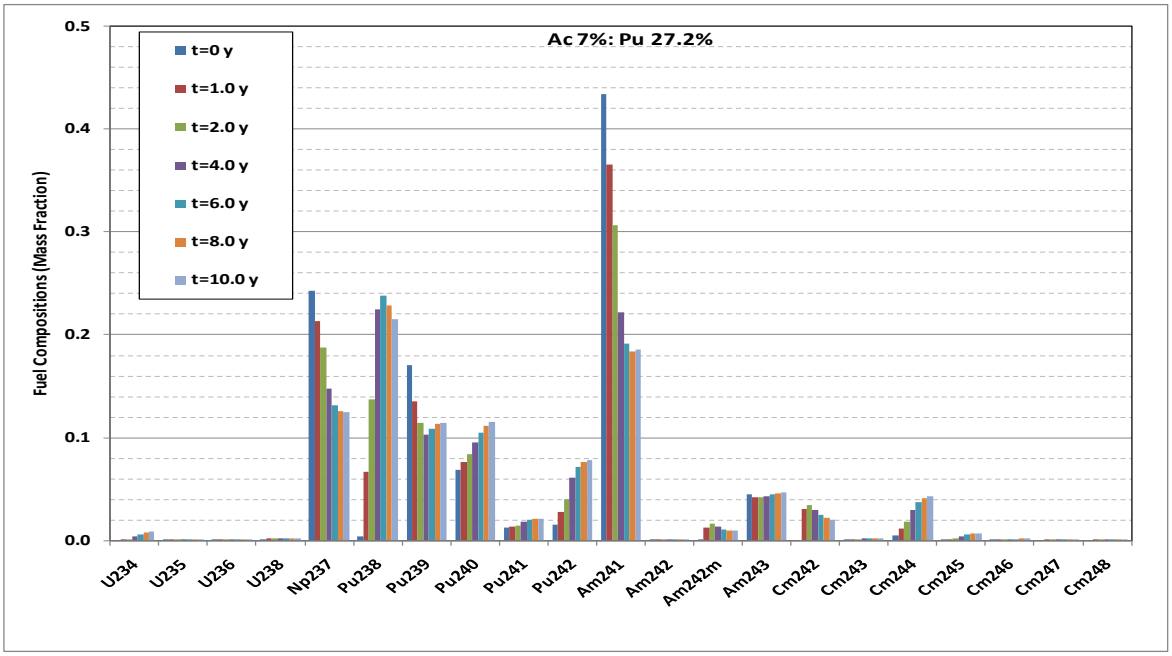


Figure 23 Actinide isotopic compositions during first 10 burnup years for blanket configuration 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides.

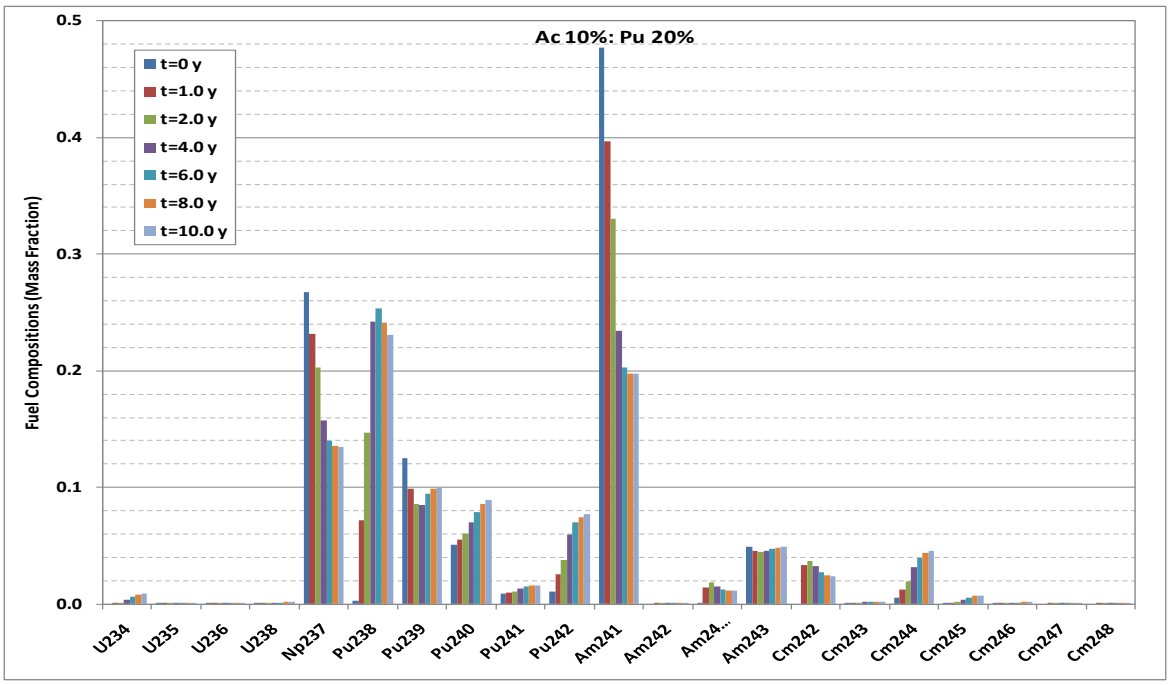


Figure 24 Actinide isotopic compositions during first 10 burnup years for blanket configuration 10% actinide concentration in LBE and 20% plutonium concentration in actinides.

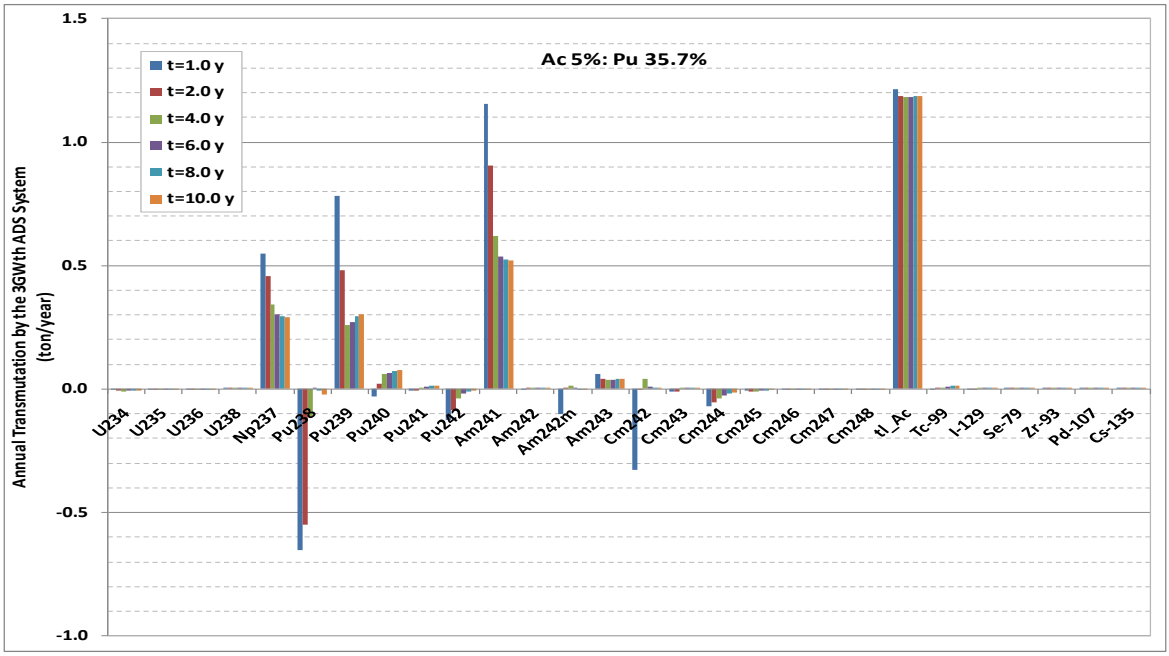


Figure 25 Annual transmutation rates of actinide isotopes and LLFPs isotopes during first 10 burnup years for blanket configuration 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides.

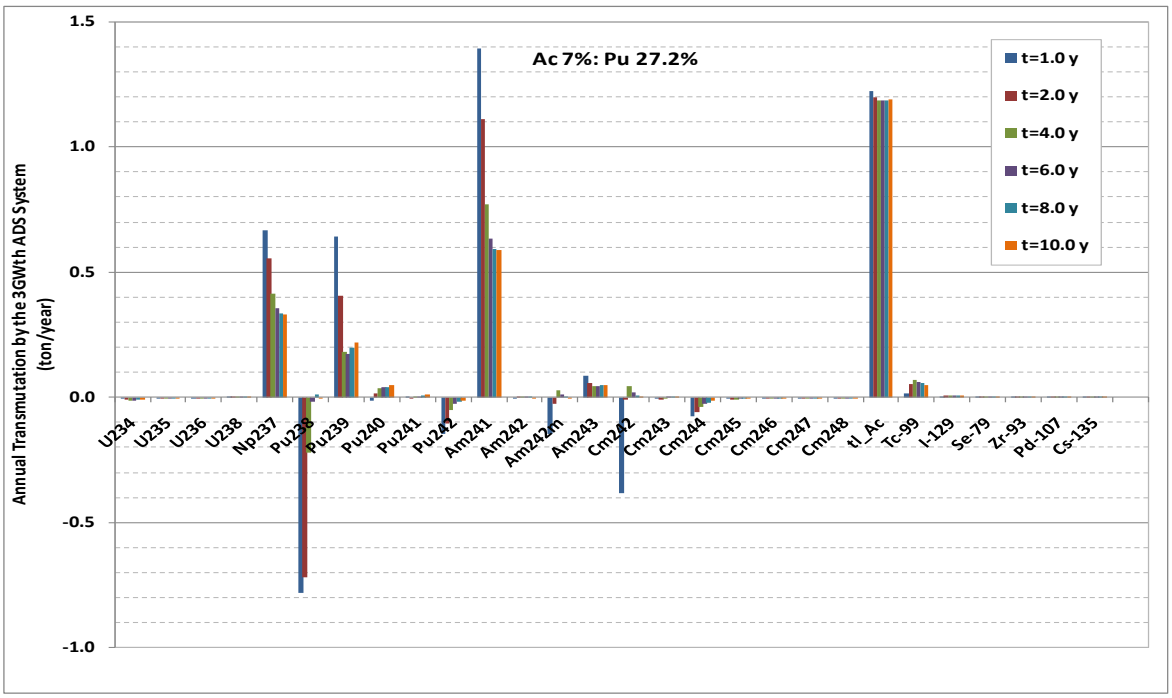


Figure 26 Annual transmutation rates of actinide isotopes and LLFPs isotopes during first 10 burnup years for blanket configuration 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides.

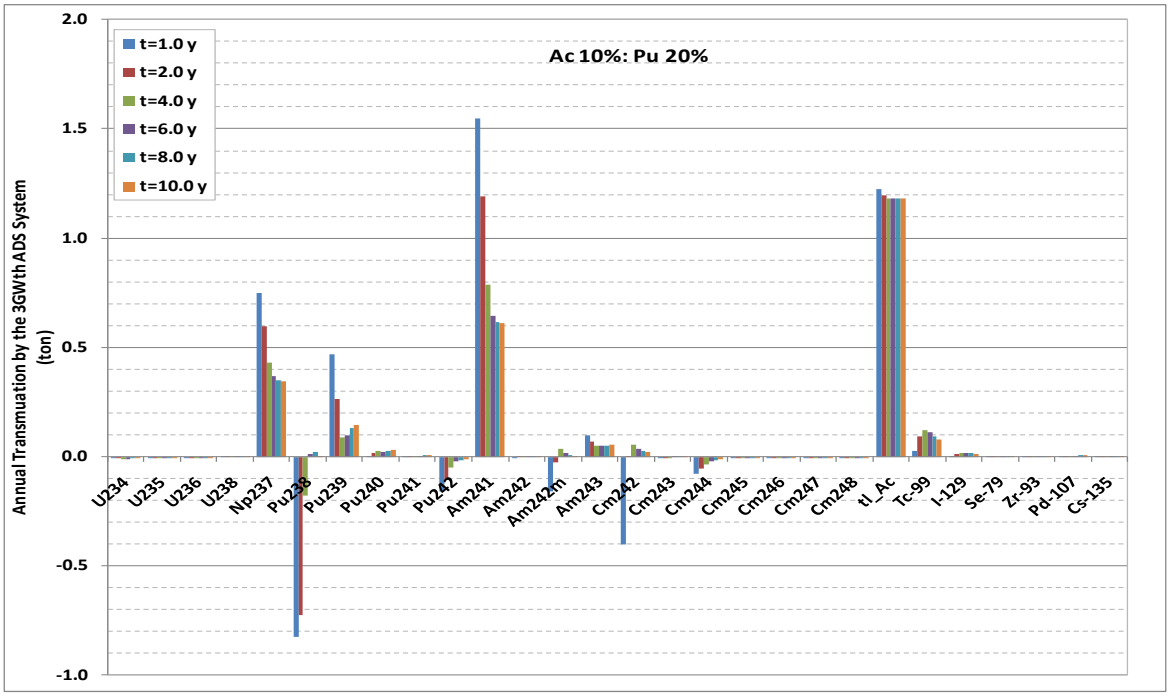


Figure 27 Annual transmutation rates of actinide isotopes and LLFPs isotopes during first 10 burnup years for blanket configuration 10% actinide concentration in LBE and 20% plutonium concentration in actinides.

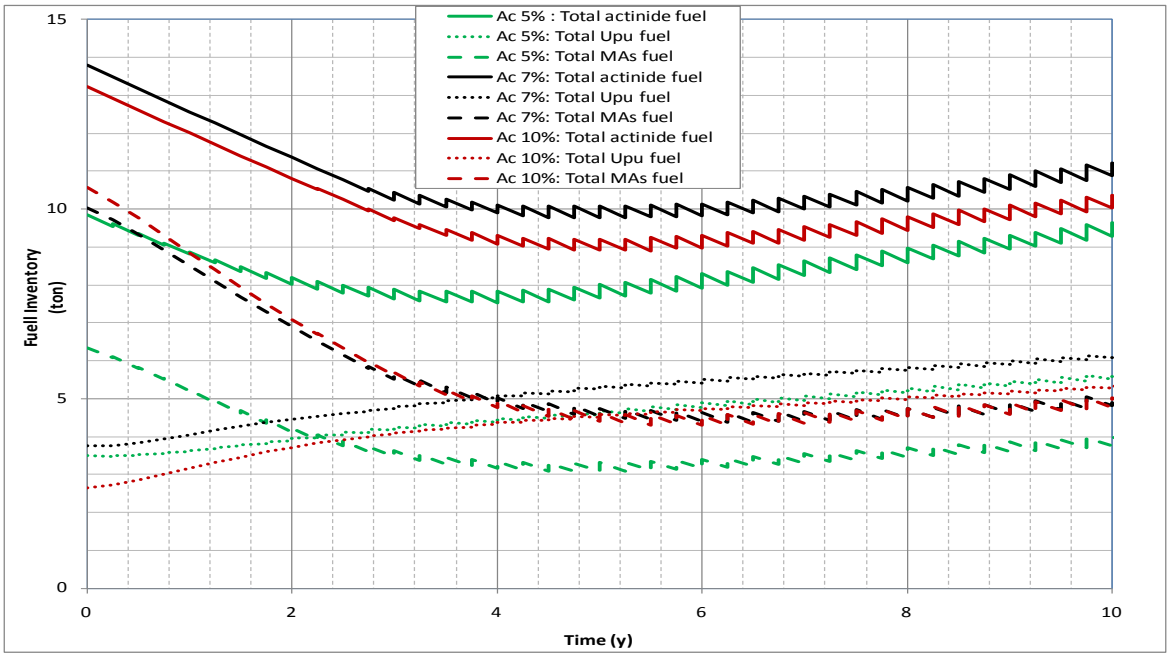


Figure 28 Actinides, U-Pu, and MAs inventories at each time-step during first 10 burnup years for the three blanket configurations of Table IV.

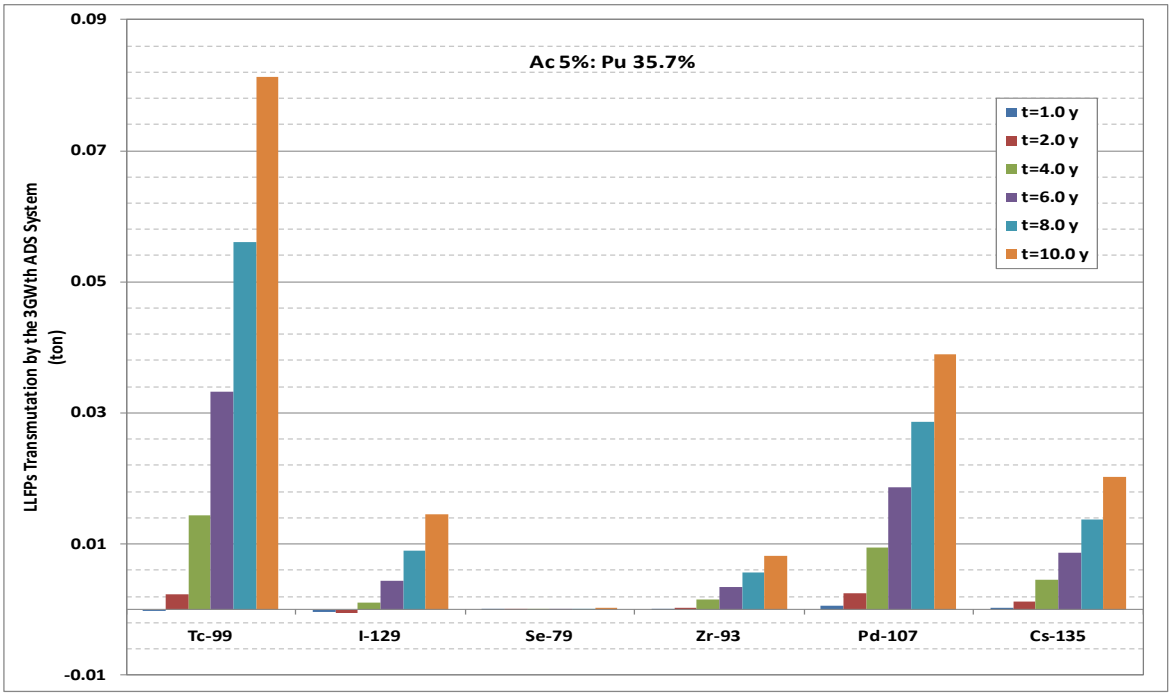


Figure 29 LLFPs consumption during first 10 burnup years for blanket configuration with 5% actinide concentration in LBE and 35.7% plutonium concentration in actinides.

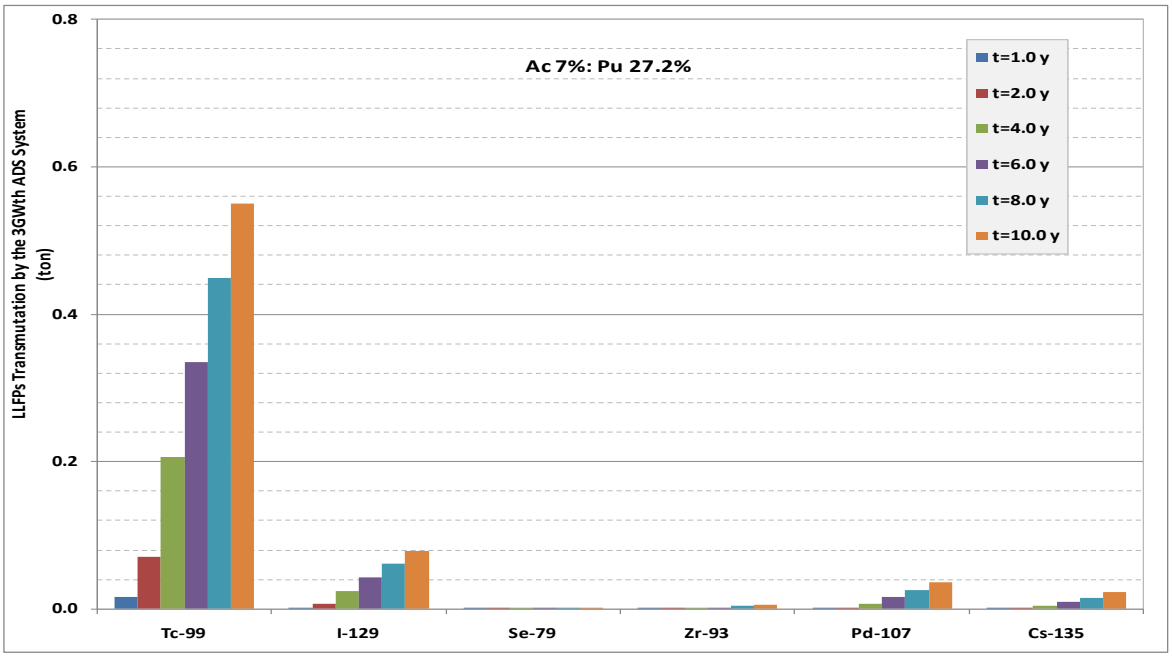


Figure 30 LLFPs consumption during first 10 burnup years for blanket configuration with 7% actinide concentration in LBE and 27.2% plutonium concentration in actinides.

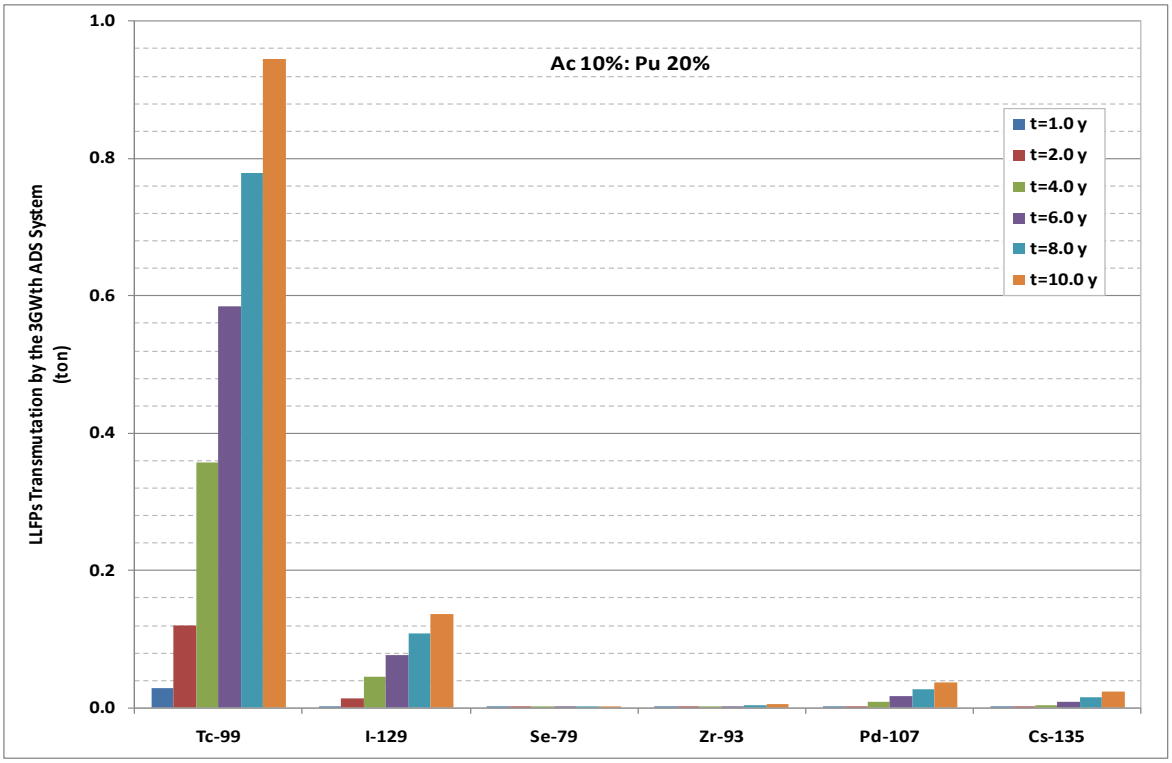


Figure 31 LLFPs consumption during first 10 burnup years for blanket configuration with 10% actinide concentration in LBE and 20% plutonium concentration in actinides.

Appendix A: Discrete Feeding Factor Estimate

The following procedure is used to estimate the amount of feeding materials required at the end of each burnup time-step. The feeding amount is intended to adjust the effective neutron multiplication factor to the value at the beginning of the burnup time-step. First, at the beginning of the step t = 0, the Boltzmann equation can be represented as

$$L_0\phi_0 = \frac{1}{k_0}(\chi F)_0\phi_0. \tag{3}$$

Where L and (χF) are the neutron destruction and neutron production operators, respectively, k_0 is the eigenfunction or the neutron multiplication factor. The Boltzmann equation at the end the time-step $t = t_1$ is

$$L_1\phi_1 = \frac{1}{k_1}(\chi F)_1\phi_1. \tag{4}$$

The objective of adding feeding materials to the system is to let the new system achieve

$$(L_1 + \Delta L)\phi' = \frac{1}{k_0}\left[(\chi F)_1 + \Delta(\chi F)\right]\phi'. \tag{5}$$

Where ΔL and $\Delta(\chi F)$ are the variations of the neutron destruction and neutron production operators due to the feeding materials.

If, assuming the neutron fluxes in the fission blanket do not change significantly after the one burnup step and also after the material feeding, i.e., $\phi_0 \sim \phi_1 \sim \phi'$, the left part of Eq. 5 can be approximately as

$$(L_1 + \Delta L)\phi' \cong L_1\phi_1 + \Delta L\phi = \frac{1}{k_1}(\chi F)_1\phi_1 + \Delta L\phi. \tag{6}$$

Eq. 5 can then be rearranged into

$$\left(\frac{1}{k_1} - \frac{1}{k_0}\right)(\chi F)_1\phi_1 \cong \frac{1}{k_0}\Delta(\chi F)\phi_1 - \Delta L\phi_1. \tag{7}$$

To calculate ΔL and $\Delta(\chi F)$, it is assumed that the atom compositions of the feeding vector is fixed and that only the total amount of feeding material varies:

$$\Delta N_{i,j} = f_j N_{i,0}, \quad i \in \text{feed vector} \tag{8}$$

where f_j is the feeding factor at the end of the jth time-step, $\Delta N_{i,j}$ is the atom densities of the ith isotope in the feeding vector adding into the fission blanket at the end of the jth time step, and $N_{i,0}$ is the fixed atom density for the ith isotope in the feeding vector. Therefore, the neutron destruction and production operator can be calculated as

$$\frac{1}{k_0}\Delta(\chi F)\phi_1 = \frac{f}{k_0}\sum_i \chi_i \sigma_{f,i} N_{i,0}\phi_1, \tag{9}$$

and

$$\Delta L \phi_1 = f\sum_i \sigma_{r,i}\phi_1 N_{i,0} - \sum_{i \in FPgas} \sigma_{r,i} N_i \phi_1. \tag{10}$$

The feeding factor f can then be estimated to be

$$f = \frac{\left(1/k_1 - 1/k_0\right)\sum_i \chi_i \sigma_{f,i} N_{i,1}\phi_1 - \sum_{i \in FPgas} \sigma_{r,i} N_i \phi_1}{1/k_0 \sum_i \chi_i \sigma_{f,i} N_{i,0}\phi_1 - \sum_i \sigma_{r,i} N_{i,0}\phi_1}. \tag{11}$$

In the Eq. 11, the microscopic reaction rates are approximated with the reaction rates calculated by MCB5 fixed-source problem, and the multiplication factors k_0 and k_1 are from the MCB5 eigenvalue calculations.

Appendix B: Computer Script Codes

B.1 Python job script to calculate feed factor *f* of Appendix A

```
#! /usr/bin/env python

# clean the liquid, FP noble gas immediately removed
# and all assume 10% liquid is cleaned (10% FPs is removed)

import os, glob, pickle
Ac_list=[['U234','92234'],['U235','92235'],['U236','92236'],['U237','92237'],\
        ['U238','92238'],['U239','92239'],['U233','92233'],['U232','92232'],\
        ['Np237','93237'],['Np238','93238'],\
        ['Pu238','94238'],['Pu239','94239'],['Pu240','94240'],['Pu241','94241'],\
        ['Pu242','94242'],['Pu243','94243'],['Pu244','94244'],\
        ['Am241','95241'],['Am242','95242'],['Am242m','95342'],['Am243','95243'],\
        ['Cm242','96242'],['Cm243','96243'],['Cm244','96244'],['Cm245','96245'],\
        ['Cm246','96246'],['Cm247','96247'],['Cm248','96248']]
Initial_nofuel_list=[['O16','8016'],['Pb206','82206'],['Pb207','82207'],\
                    ['Pb208','82208'],['Bi209','83209']]
FP_gas_list=[['Kr80','36080',0.0], ['Kr82','36082',0.0], ['Kr83','36083',0.0],
['Kr84','36084',0.0],\
           ['Kr85','36085',0.0], ['Kr86','36086',0.0], \

['Xe124','54124',0.0],['Xe126','54126',0.0],['Xe128','54128',0.0],['Xe129','54129',0.0],\

['Xe130','54130',0.0],['Xe131','54131',0.0],['Xe132','54132',0.0],['Xe133','54133',0.0],\
           ['Xe134','54134',0.0],['Xe135','54135',0.0],['Xe136','54136',0.0]]
FP_LL_list=[['Se79','34079', 0.0],['Zr93','40093', 0.0],['Tc99','43099',0.8512 ],\
          ['Pd107','46107',0.0],['I129','53129', 0.1488]]

fBVol=0.0
# read the actinide fuel feeding vector
fr0=open('inp0','r')
feed_vector_Ac=[]
line = fr0.readline()
while line > '':
   if line.find('BVOL') >=0:
      fBVol = float(line.split()[1])
   if line.find('nlib = 72c') >=0:
      line = fr0.readline()
      while line.find('.72c') >=0:
         feed_vector_tmp =[]
         linesplit = line.split()
         Istptmp = linesplit[0].split('.72c')[0]
```

```
        if int(Istptmp) > 90000:
          for x in Ac_list:
              if x[1]== Istptmp :
                feed_vector_tmp.append(x[0])
                break
              feed_vector_tmp.append(Istptmp)
              Density = float(linesplit[1])
              feed_vector_tmp.append(Density)
              feed_vector_Ac.append(feed_vector_tmp)
        line=fr0.readline()
    else:
      line=fr0.readline()

fr0.close()
```

```
# calculate macroscopic reaction rate terms in the numerator:
# chifission, capture due to the fpgas, capture due to the other fps

fr=open('fission_rates', 'r')
micro_fis_rate=[]
for line in fr:
    rct_rate_tmp=[]
    linesplit = line.split()
    if linesplit[0].count('.72c') == 0:
      rct_rate_tmp.append(linesplit[0])
      rct_rate_tmp.append(float(linesplit[3]))
      rct_rate_tmp.append(float(linesplit[5]))
      micro_fis_rate.append(rct_rate_tmp)
    else:
      rct_rate_tmp.append(linesplit[0].split('.')[0])
      rct_rate_tmp.append(float(linesplit[2]))
      rct_rate_tmp.append(float(linesplit[4]))
      micro_fis_rate.append(rct_rate_tmp)
fr.close()

# read micro_cap_rates
fr=open('capture_rates','r')
micro_cap_rate=[]
for line in fr:
    rct_rate_tmp=[]
    linesplit = line.split()
    if linesplit[0].count('.72c') == 0:
      rct_rate_tmp.append(linesplit[0])
      rct_rate_tmp.append(float(linesplit[3]))
      micro_cap_rate.append(rct_rate_tmp)
    else:
```

```
        rct_rate_tmp.append(linesplit[0].split('.')[0])
        rct_rate_tmp.append(float(linesplit[2]))
        micro_cap_rate.append(rct_rate_tmp)
fr.close()

fChi = 3.0197

# 39alamo39g39 the reaction rates at the end of the burnup step
fr=open('mass_total','r')
# macroscopic chifission reaction rates
sum_1_fis=0.0
# macroscopic capture reaction rates for non-gas-FPs, gas FPs
sum_1_cap_FPs=0.0
sum_1_cap_Fpgas=0.0
# calculate the fission reaction rates after burnup
for line in fr:
        linesplit=line.split()
        Istptmp = linesplit[0].split('_')[1].split('=')[0]
        mass_1 = float(linesplit[2].split(']')[0])
        iflag = 0
        for x in micro_fis_rate:
            if Istptmp == x[0]:
                iflag=iflag+1
                if iflag == 2:
                    lnth = len(Istptmp)
                    istmp1=''
                    for i in range(0,lnth):
                        if Istptmp[i] < 'A':
                            istmp1=istmp1+Istptmp[i]
                    istp_mass = int(istmp1)
                    sum_1_fis = sum_1_fis + mass_1 / istp_mass / fBVol * 0.6023 * x[1] * fChi
 #                    print 'fuel actinide isotope:',Istptmp
                    break
        if iflag == 0:
           for x in Initial_nofuel_list:
                if Istptmp == x[0]:
                   iflag = iflag +1
#                    print 'input none fuel isotope:', Istptmp
                   break
           if iflag == 0:
              for x in micro_cap_rate:
                 if Istptmp == x[0]:
                    iflag=iflag+1
                    if iflag == 2:
                       lnth = len(Istptmp)
                       istmp1=''
                       for i in range(0,lnth):
```

```
                    if Istptmp[i] < 'A':
                        istmp1=istmp1+Istptmp[i]
                istp_mass = int(istmp1)
                iflagy=0
                for y in FP_gas_list:
                    if Istptmp == y[0]:
                        sum_1_cap_Fpgas = sum_1_cap_Fpgas + mass_1 / istp_mass /
fBVol * 0.6023 * x[1]
                        iflagy=iflagy+1
  #                       print 'Fission gas', Istptmp
                        break;
                if iflagy == 0:
   #                    print 'Fission Product', Istptmp
                    sum_1_cap_FPs = sum_1_cap_FPs + mass_1 / istp_mass / fBVol *
0.6023 * x[1]
                    break
fr0.close()
```

```
# calculate the macroscopic reaction rate terms in the denominator:
# chifission, capture

# read the eigenvalue before and after the burnup
fr=open('keff_1','r')
fKeff=[]
for lines in fr:
    index=lines.find('keff =')
    line1 = lines[index:len(lines)]
    fKeff.append(float(line1.split()[2]))
fr.close()
fDeltaKeff = fKeff[1] – fKeff[0]

# fDeltaKeff >0, feed with LLFPs
# otherwise, feed with the actinide fuels
sum_0_fis = 0.0
sum_0_cap = 0.0

feed_vector=[]
if fDeltaKeff > 0 :
  feed_vector = FP_LL_list
  for y in feed_vector:
      iflag = 0
      for x in micro_cap_rate:
          if y[0] == x[0] :
             iflag = iflag +1
             if iflag == 2:
                sum_0_fis = 0
```

```
            sum_0_cap =  sum_0_cap + y[2] * x[1]
            break
else:
  feed_vector = feed_vector_Ac
  for y in feed_vector:
     iflag = 0
     for x in micro_fis_rate:
        if y[0] == x[0]:
          iflag = iflag + 1
          if iflag == 2:
            sum_0_fis = sum_0_fis + y[2] * fChi * x[1]
            sum_0_cap = sum_0_cap + y[2] * x[2]
            break
```

```
# fDeltaKeff >0 feed_factor is the total atom density of the feed LLFPs
# otherwise, feed_factor is the percentage of the feed actinide fuels compared with the
initial fuel inventory in LBE
# FP gas is completely removed, other FPs is partially removed due to liquid
41alamo41g process
# FP_factor: the percentage of FPs left in the LBE
FP_factor = 0.9
Feed_factor = (-(fKeff[1]-0.980)/fKeff[1]/fKeff[0] * sum_1_fis – sum_1_cap_Fpgas –
sum_1_cap_FPs*(1-FP_factor) ) / (sum_0_fis/fKeff[0] – sum_0_cap)
#   Feed_factor = (-(fKeff[1]-0.980)/fKeff[1]/fKeff[0] * sum_1_fis – sum_1_cap) /
(sum_0_fis/fKeff[0] – sum_0_cap)
#   Feed_factor = (-(fKeff[1]-0.980)/fKeff[1]/fKeff[0] * sum_1_fis) / (sum_0_fis/fKeff[0] –
sum_0_cap)

if Feed_factor < 0.0:
  Feed_factor = 0.0  # the removal of FPs compenstated the Keff loss

fr0=open('Feed_factor_vector','a')
fr0.write(str(Feed_factor))
fr0.write('\n')
pickle.dump(feed_vector,fr0)
fr0.write('\n')
fr0.close()
```

```
# adjust the atom densities
# step 1, read and calculate the atom densities at the end of burnup step
fr0=open('minp','r')
atom_density=[]
lines = fr0.readline()
while lines > '':
   if lines.find('Fission blanket') >=0:
     lines=fr0.readline()
```

```
        density =lines.split('atomic density')[1].split('[')[0]
        density=density.lstrip()
        density=density.rstrip()
        tot_atom_density=float(density)
    if lines.find('nlib') >=0:
        index1 = lines.find('M')
        index_mat = int(lines[index1+1:lines.find(' ',index1+1)])
        lines = fr0.readline()
        while lines.find('.72c') >0:
            linesplit = lines.split()
            for strtmp in linesplit:
                if strtmp.find('E') < 0 :
                    atom_density_tmp=[]
                    atom_density_tmp.append(strtmp)
                else:
                    atom_density_tmp.append(strtmp)
                    atom_density.append(atom_density_tmp)
            lines = fr0.readline()
    else:
        pass
    lines = fr0.readline()
fr0.close()

print atom_density
# step 2:
# adjusting the isotope atom densities
sum_atom_den=0
atom_density_modify=[]
for x in atom_density:
    iFlag=0
    dentmp = float(x[1]) * tot_atom_density
    print x
    for y in feed_vector:
        if x[0].find(y[1]) >=0:
            dentmp = dentmp + Feed_factor * y[2]
            sum_atom_den = sum_atom_den + dentmp
            x[1] = str(dentmp)
            atom_density_modify.append(x)
            iFlag = iFlag +1
            print 'Feeding isotopes adjusted:', x, y
            break
    if iFlag == 0:
        for y in FP_gas_list:
            if x[0].find(y[1])>=0:
                iFLag = iFlag + 1
                print 'FP gas passed', x, y
                break
```

```
        if iFlag == 0:
          for y in Initial_nofuel_list:
             if x[0].find(y[1]) >=0:
                sum_atom_den = sum_atom_den + dentmp
                x[1] = str(dentmp)
                atom_density_modify.append(x)
                iFlag = iFlag + 1
                print ‘initial none fuel isotope :’, x, y
                break
          if iFlag == 0:
            istmp = int(x[0].split(‘.72c’)[0])
            if istmp < 90000:
              dentmp = dentmp * FP_factor
              if dentmp > 0:
                sum_atom_den = sum_atom_den + dentmp
                x[1] = str(dentmp)
                atom_density_modify.append(x)
                print ‘FP products adjusted:’, x
              else:
                print ‘FP products passed’, x
            else:
              print ‘actinides no adjustment:’,x
              sum_atom_den = sum_atom_den + dentmp
              x[1] = str(dentmp)
              atom_density_modify.append(x)

# prepare the input file for next step k-eigenvalue calculation
fr0 = open(‘inp’,’w’)
fr1 = open(‘inp0’,’r’)
lines = fr1.readline()
while lines > ‘’:
   if lines.find(‘Fission blanket’) >=0:
      strline = lines
      fr0.write(strline)
      lines= fr1.readline()
      linesplit = lines.split()
      index1=lines.find(linesplit[2])
      index2 = lines.find(‘ ‘, index1+1)
      strline = lines[0:index1] + str(sum_atom_den) + lines[index2:len(lines)-1] + ‘\n’
      fr0.write(strline)
      lines =fr1.readline()
   elif lines.find(‘SSR’) >= 0:
      strline =’c ‘+ lines
      fr0.write(strline)
      lines=fr1.readline()
   elif lines.find(‘nps’) >=0:
      strline = ‘c ‘+lines
```

```
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('BURN') >=0:
    strline = 'c '+lines
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('BVOL') >=0:
    strline = 'c '+lines
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('BATCT') >=0:
    strline = 'c '+lines
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('DISCR') >=0:
    strline = 'c '+lines
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('PRIOD') >=0:
    strline = 'c '+lines
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('POWER') >=0:
    strline = 'c '+lines
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('NOFP') >=0:
    strline = 'c '+lines
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('AFTER') >=0:
    strline = 'c '+lines
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('INPRT') >=0:
    strline = 'c '+lines
    fr0.write(strline)
    lines=fr1.readline()
elif lines.find('nlib') >= 0:
    strline = lines
    fr0.write(strline)
    lines = fr1.readline()
    while lines.find('.72c') >=0:
        lines = fr1.readline()
    for x in atom_density_modify:
        strline ='       '+ x[0] + '    ' + x[1] + '\n'
        fr0.write(strline)
```

```
    else:
        strline = lines
        fr0.write(strline)
        lines = fr1.readline()

fr0.close()
fr1.close()
```

B.2 Python job script to adjust feed factor *f*

```
#! /usr/bin/env python

import os, glob, pickle

# read keff for the new BOL, adjusting the feeding factor such that keff~0.98
fr=open('keff_2','r')
lines=fr.readline()
index=lines.find('keff =')
line1 = lines[index:len(lines)]
fKeff=float(line1.split()[2])
if (fKeff – 0.98) > 0.001:
   fAdjustFactor = 1- abs(fKeff – 0.98) / 0.0025* 0.1
elif (fKeff – 0.98) < - 0.001:
   fAdjustFactor = 1 + abs(fKeff – 0.98) / 0.0025 * 0.1
else:
   fAdjustFactor = 1.0

print fAdjustFactor

# read feeding factor and feeding vector, burnup zone volume
fr0=open('Feed_factor_vector','r')
Feed_factor = float(fr0.readline());
feed_vector = pickle.load(fr0)
fr0.close()

# Adjust feeding factor

fr0=open('inp','r')
atom_density=[]
lines = fr0.readline()
while lines > '':
    if lines.find('nlib') >=0:
        index1 = lines.find('M')
        index_mat = int(lines[index1+1:lines.find(' ',index1+1)])
        lines = fr0.readline()
        while lines.find('.72c') >0:
```

```
        linesplit = lines.split()
        print lines, linesplit
        atom_density_tmp=[]
        atom_density_tmp.append(linesplit[0])
        atom_density_tmp.append(linesplit[1])
        atom_density.append(atom_density_tmp)
        lines = fr0.readline()
    else:
      pass
    lines = fr0.readline()
fr0.close()

# adjusting the isotope atom densities

sum_atom_den=0
atom_density_modify=[]
for x in atom_density:
     dentmp = float(x[1])
     iFlag=0
     for y in feed_vector:
        if x[0].find(y[1]) >=0:
           dentmp = dentmp – Feed_factor * y[2]*(1-fAdjustFactor)
           sum_atom_den = sum_atom_den + dentmp
           x[1] = str(dentmp)
           atom_density_modify.append(x)
           print ‘Feeding isotopes adjusted:’, x, y
           iFlag = iFlag +1
           break
     if iFlag == 0:
       sum_atom_den = sum_atom_den + dentmp
       atom_density_modify.append(x)
     else:
       pass

# creat a new input file for testing the keff
fr0 = open(‘inp’,’w’)
fr1 = open(‘inp0’,’r’)
lines = fr1.readline()
while lines > ‘’:
    if lines.find(‘Fission blanket’) >=0:
      strline = lines
      fr0.write(strline)
      lines= fr1.readline()
      linesplit = lines.split()
      index1=lines.find(linesplit[2])
      index2 = lines.find(‘ ‘, index1+1)
      strline = lines[0:index1] + str(sum_atom_den) + lines[index2:len(lines)-1] + ‘\n’
```

```
      fr0.write(strline)
      lines =fr1.readline()
    elif lines.find('nlib') >= 0:
      strline = lines
      fr0.write(strline)
      lines = fr1.readline()
      while lines.find('.72c') >=0:
        lines = fr1.readline()
      for x in atom_density_modify:
          strline ='       '+ x[0] + '     ' + x[1] + '\n'
          fr0.write(strline)
    else:
      strline = lines
      fr0.write(strline)
      lines = fr1.readline()

fr0.close()
fr1.close()
```

B.3 Shell script to run MCB5 code

```
#!/bin/bash
#
#PBS –N MCB5_cnst_feed
#PBS –l nodes=8:ppn=8
#PBS –l walltime=96:00:00
#PBS –j oe
#PBS –V
#PBS –S /bin/bash
#PBS –o /home/cluster3/ycao/ADS SYSTEM/ENDFB7/Ac7/FPs_90/
#PBS –e /home/cluster3/ycao/ADS SYSTEM/ENDFB7/Ac7/FPs_90/

export MPIR_HOME=/home/cluster1/47alamo/src/mpich2-1.3.1-prefix/
ulimit –s unlimited

mcb=/home/cluster3/zzhong/MCB5/src/MCNP5_32B_Am/Source/src/mcb5.mpi
NSLOTS=`cat $PBS_NODEFILE | wc –l`
NNODES=`expr $NSLOTS / 8`
cat $PBS_NODEFILE

cd  $PBS_O_WORKDIR

for i in 1 2 3 4 5 6 7 8 9 10
do

if [ "$i" –le "1" ]
```

```
 then
cp inp inp0
fi

mkdir $$
cd $$
export INPUT=inp
export INP0=inp0
export myscript_1=myscript1.py
export myscript_2=myscript2.py
export srctp=srctp_Am

cp $PBS_O_WORKDIR/$INPUT inp
cp $PBS_O_WORKDIR/$INP0 inp0
cp $PBS_O_WORKDIR/srctp_Am srctp
cp $PBS_O_WORKDIR/$myscript_1 myscript_1.py
cp $PBS_O_WORKDIR/$myscript_2 myscript_2.py

ln –s
/home/cluster1/48alamo/XSLIB/ascii/ENDFB7+JEFF3.1+IRDF2002+ENDFB6.8_MCBLA
BELS.xsdir xsdir
ln –s /home/cluster3/ycao/ADS SYSTEM/ENDFB7/rssa_fusion rssa

$MPIR_HOME/bin/mpirun –np $NSLOTS –machinefile $PBS_NODEFILE $mcb

mv inp inp_$i
grep '.72c    -6' bmes > fission_rates
grep '.72c   102' bmes > capture_rates
grep 'tot_' btab > mass_total
grep 'the final estimated combined collision' outp > keff_1
rm runtpe
rm for*

myscript_1.py
$MPIR_HOME/bin/mpirun –np $NSLOTS –machinefile $PBS_NODEFILE $mcb
grep 'the final estimated combined collision' outp > keff_2

myscript_2.py
cp inp $PBS_O_WORKDIR/inp
cp btab $PBS_O_WORKDIR/btab_$i
mv srctp $PBS_O_WORKDIR/$srctp
rm runtpe
rm fort*

cd $PBS_O_WORKDIR
mv $$ step_$i
done
```

Nuclear Engineering Division
Argonne National Laboratory
9700 South Cass Avenue, Bldg. 208
Argonne, IL 60439

www.anl.gov

A U.S. Department of Energy laboratory
managed by UChicago Argonne, LLC