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A COMPARATIVE STUDY OF MONTEBURNS AND MCNPX 2.6.0 CODES IN ADS SIMULATIONS

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ABSTRACT

The possible use of the MONTEBURNS and MCNPX 2.6.0 codes in Accelerator-driven systems (ADSs) simulations for fuel evolution description is discussed. ADSs are investigated for fuel breeding and long-lived fission product transmutation so simulations of fuel evolution have a great relevance. The burnup/depletion capability is present in both studied codes. MONTEBURNS code links Monte Carlo N-Particle Transport Code (MCNP) to the radioactive decay burnup code ORIGEN2, whereas MCNPX depletion/ burnup capability is a linked process involving steady-state flux calculations by MCNPX and nuclide depletion calculations by CINDER90. A lead-cooled accelerator-driven system fueled with thorium was simulated and the results obtained using MONTEBURNS code and the results from MCNPX 2.6.0 code were compared. The system criticality and the variation of the actinide inventory during the burnup were evaluated and the results indicate a similar behavior between the results of each code.

1. INTRODUCTION

In recent years great interest has been displayed for accelerator-driven subcritical reactors (ADS) to produce energy, transmute radioactive wastes and fertile to fissile fuel conversion in a cleaner and safer way than at present. Pioneers in this revival have been Furukawa [1], Bowman [2] and Rubbia [3]. Similar ideas were proposed almost 50 years ago [4–7].

The concept of ADS combines a particle accelerator with a subcritical core, in general, an ADS consists of three parts: (1) accelerator, (2) spallation neutron target and (3) sub-critical core. A high intensity proton beam with energy of around 1 GeV is injected into a target of heavy metal, resulting in spallation reactions that emit neutrons. The spallation process is a nuclear reaction where high-energy particles hit target nuclei of heavy elements. The main purpose of spallation target in an ADS is to provide the primary neutron flux for driving the fission process in the subcritical core.

The feasibility of thorium utilization in ADS has been investigated [8-10]. There are many reasons for the resurgence of interest in the thorium fuel cycle nowadays. Thorium is about

three times more abundant than uranium abundance and is distributed in nature as an easily exploitable resource in many countries. The main issue verified in the adoption of this fuel is the initial enrichment requirement, since the use of natural thorium (^{232}Th) is not feasible due to the very low values of achieved criticality.

Multiple computer codes have been used to model ADS cores designed for the purpose of burning fuels. The fuel evolution description is essential when it is desired to know fuel breeding performance. In the present study, it was performed a comparison of MCNPX 2.6.0 [11] and MONTEBURNS 2.0 [12] codes on an ADS fueled with thorium simulation. MCNPX depletion/ burnup capability is a linked process involving steady-state flux calculations by MCNPX and nuclide depletion calculations by CINDER90. During the burnup the MCNPX does not take into account the flux from external source, so the effective neutron multiplication factor ($k_{eff)}$ and fuel evolution results obtained in an ADS simulation with MCNPX are just approximations. MONTEBURNS code links Monte Carlo N-Particle Transport Code (MCNP) to the radioactive decay burnup code ORIGEN2. Monteburns produces a large number of criticality and burnup results based on various material feed/removal specifications, power(s), and time intervals. In MONTEBURNS the value of the effective multiplication factor for an external source definition (spallation source) must be calculated, so the flux from spallation source is take into account in an ADS simulation.

In summary, this computational study aims to determine the difference between the results obtained using MONTEBURNS code and the results from MCNPX 2.6.0 in a lead-cooled accelerator-driven system fueled with thorium simulation. A comparison of the results obtained from each code allows verifying when it is considered the neutron flux from the spallation source during the operation period. The system criticality, the neutron spectrum and the variation of the actinide inventory during the burnup were evaluated and the results indicate a similar behavior between the results provide by each code.

2. METHODOLOGY

2.1. System Parameters

Fig. 1 shows schematic views of the simulated ADS in MCNPX and MONTEBURNS. The codes share the same MCNP geometry. The basic geometry includes the lead spallation target, a subcritical core, and the reflector. The accelerator tube has a radius of 1.5 cm, and the axial position is in the center of the target. The spallation source is represented by a neutrons source with a spectrum characteristic of spallation reactions. Such spectrum was generated, in a previous simulation, using a beam of 1-GeV protons with a parabolic spatial profile. There was used Bertini intranuclear cascade model for the transport of protons, neutrons, and charged pions. The parameters of this simulation were described in [13].

Due to their higher neutron yields only heavy targets are considered practical. Lead or lead-bismuth, are proposed as liquid targets. The use of only lead for the target prevents the radiological hazards from ^{210}Po, maintaining a high neutrons production by spallation, since the values of spallation cross sections for the two materials are very close.

The core is a cylinder of 6.0 m^3 filled with a hexagonal lattice loaded with a mixture of $^{232}ThO_2$ + 15% $^{233}UO_2$. The volumetric fractions of coolant (54 %) and fuel (8 %) were adjusted to obtain initial k_{eff} = 0.99. The inner diameter of the 156 fuel rods is 2. The coolant used is natural Lead. This design offers many advantages like convective cooling, passive safety and small neutron absorption cross section [14].

Another advantage of the lead coolant is that it is not a neutron moderator. This is important because the protactinium effect, which limits the achievable values of k_{eff}, is less severe for harder spectra. For solid fuels, systems without moderator and based on thorium, smaller values of capture cross sections of fission products will reduce the k_{eff} variation and produce a hardening (shift to higher energies) in the neutron energy distribution. So, the inventory of ^{233}U is much larger in fast reactors (about 7 times), with the associated larger breeding times and inventory radiotoxicity [15].

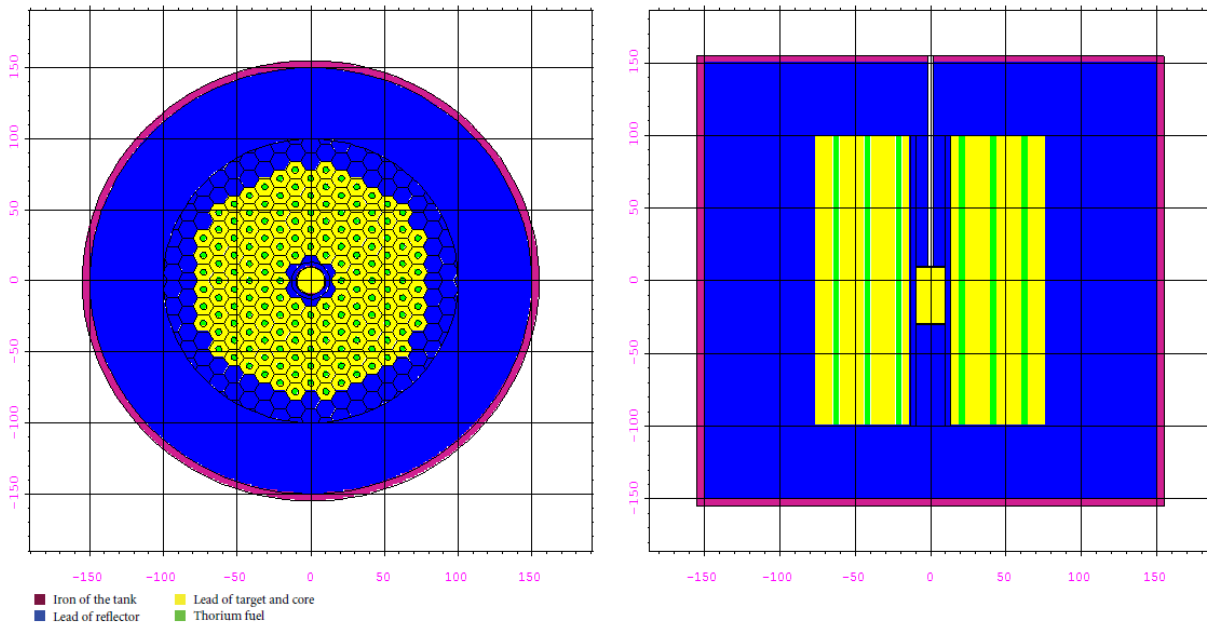

Figure 1: Horizontal and vertical cross sections of the ADS.

2.2 Computational Tools

MCNPX 2.6.0 code was used to simulate the geometrical and operational characteristics of the system. Such version is quite interesting for the ADS evaluation because it describes the nuclear fuel evolution during the operation. For the simulation there was used a combination of spallation source (external source - SDEF) and kcode-mode for the calculation of initial k_{eff} and flux, describing in this way the real behavior of an ADS; that is, the initial criticality is the sum of neutrons produced by fission in the fuel and the neutrons produced by spallation in the target. During the burnup the code does not take into account the flux from external source, so the k_{eff} and fuel evolution results obtained are just approximations. Moreover, the

k_{eff} results that were obtained during the burnup (kcode-mode) provide an insight of the necessary contribution of the external source during the operation period.

The depletion/burnup capability of MCNPX is based on CINDER90. MCNPX depletion is a linked process involving steady-state flux calculations by MCNPX and nuclide depletion calculations by CINDER90. The code runs a steady-state calculation to determine the system eigenvalue, 63-group fluxes, energy-integrated reaction rates, fission multiplicity, and recoverable energy per fission (Q values). CINDER90 then takes those MCNPX-generated values and performs the depletion calculation to generate new number densities for the next time step. MCNPX takes these new number densities and generates another set of fluxes and reaction rates. The process repeats itself until after the final time step specified by the user [16].

MONTEBURNS is a fully automated tool that links the Monte Carlo transport code MCNP with the radioactive decay and burnup code ORIGEN2. MONTEBURNS produces a large number of criticality and burnup results based on various material feed/removal specifications, power(s), and time intervals. The program processes input from the user that specifies the system geometry, initial material compositions, feed/removal specifications, and other code-specific parameters. Various results from MCNP, ORIGEN2, and other calculations are then output successively as the code runs. The principle function of MONTEBURNS is to transfer one-group cross-section and flux values from MCNP to ORIGEN2, and then transfer the resulting material compositions (after irradiation and/or decay) from ORIGEN2 back to MCNP in a repeated, cyclic fashion. [12]

In MONTEBURNS, the value of the effective multiplication factor for an “sdef” source definition (external source) must be calculated from the value of the net multiplication obtained from the MCNP [12]. Therefore, the neutron flux from spallation source (sdef) is taking into account during the burnup and the results describe the real behavior of an ADS.

2.3 Computational Procedure

It was used for the MCNPX simulation a combination of ADS source (SDEF) and kcode-mode for calculation of initial k_{eff} and flux. The SDEF source was positioned on the center of the target. It was used the continuous energy library ENDF/B-VI.6. The burnup calculations were performed in kcode-mode using 53 time steps, the total simulated time was 10 years and the thermal power of operation throughout this period was $515MW_t$. The flux averaged over a cell was calculated using the tally F4.

In the MONTEBURNS simulation was shared the same MCNP geometry, material composition, nuclear data library, core thermal power, and the same spallation source (SDEF). However, in MONTEBURNS simulation it is not necessary the use of a combination of ADS source (SDEF) and kcode-mode. Because it is possible the calculation of the effective multiplication factor for an “sdef” source definition. Therefore, the burnup calculations were performed in sdef-mode, the total simulated time was 10 years and core thermal power of $515MW_t$.

3. RESULTS

3.1 Neutronic Evaluation

Fig. 2 plots the k_{eff} evolution for both the MCNPX and MONTEBURNS codes. The k_{eff} calculated by MCNPX for the first step was 0.99129 with a relative error of 0.00040 and k_{eff} = 0.55886 with a relative error of 0.00045 for a last step. The results provided by MONTEBURNS was k_{eff} = 0.99322 with a relative error of 0.00087 for the first step and k_{eff} = 0.56770 with a relative error of 0.01701 for a last step.

Concerning the codes discrepancy, the k_{eff} values were higher for MONTEBURNS, mainly because in this case the spallation source was considered during the burnup. However, it can be noted that the difference between the k_{eff} values are smoothly small (the averaged difference between values from MONTEBURNS and MCNPX was ≈ 0.02), indicating that the MCNPX use for ADS simulations is a suitable alternative for description of this systems evolution.

The drop of the k_{eff} value is mainly due to the increased poisoning caused by the accumulation of fission products having large neutron capture cross-sections and, of course, the constant energy generation by the system.

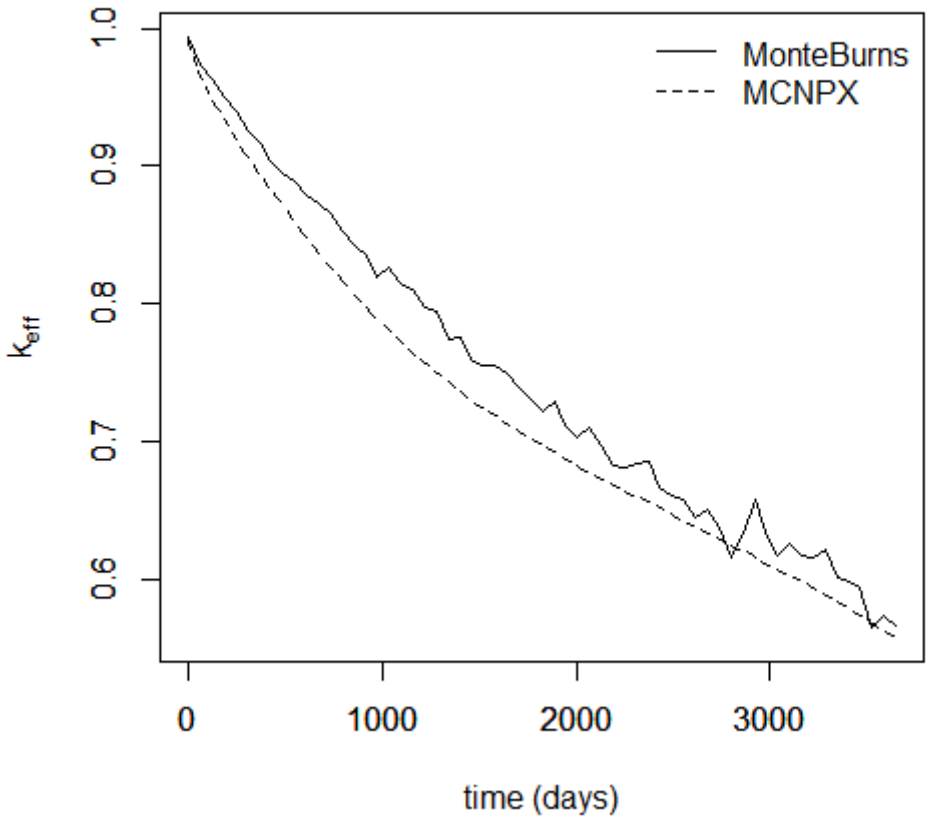

Figure 2: Multiplication factors (k_{eff}) evolution.

In Figure 3 is shown the normalized neutron flux for MCNPX simulation and the MONTEBURNS flux spectrum in the BOL (beginning of life). The normalization of the MCNPX neutron flux was performed using the flux multiplier [16]:

$$Flux\ multiplier = \frac{Power\ level\ x\ \vartheta}{Q_{value}\ x\ k_{eff}}, \qquad (1)$$

Where ν is the neutrons emitted by fission and the Q_{value} is the recoverable energy per fission

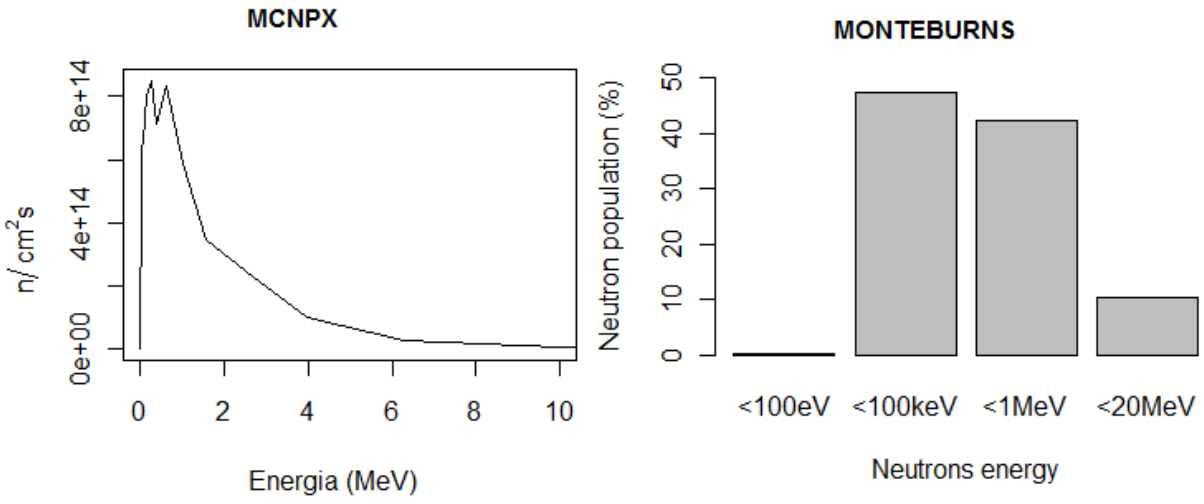

Figure 3: Neutron spectra in the beginning of life.

The maximum flux in MCNPX simulation occurred around 250 keV, the use of fast neutrons is important for the protactinium effect reduction. It can be observed a hard spectrum in MONTEBURNS simulation as well as in MCNPX simulation.

3.1 Fuel Evolution

Fig. 4 describes the ^{232}Th concentration for both the MCNPX and MONTEBURNS codes during the 10 years of operation. The consumption of ^{232}Th was very similar for both simulations. It can be verified that the concentration of this isotope is reduced by about 43% during the operation time. It is the result of the considerable capture cross section of this isotope, which allows the ^{233}U production. ^{233}U is formed when ^{232Th} captures a neutron, and it soon undergoes two beta decays:

$$^{232}\text{Th} + n \longrightarrow {}^{233}\text{Th} \xrightarrow{\beta-} {}^{233}\text{Pa} \xrightarrow{\beta-} {}^{233}\text{U} \qquad (2)$$

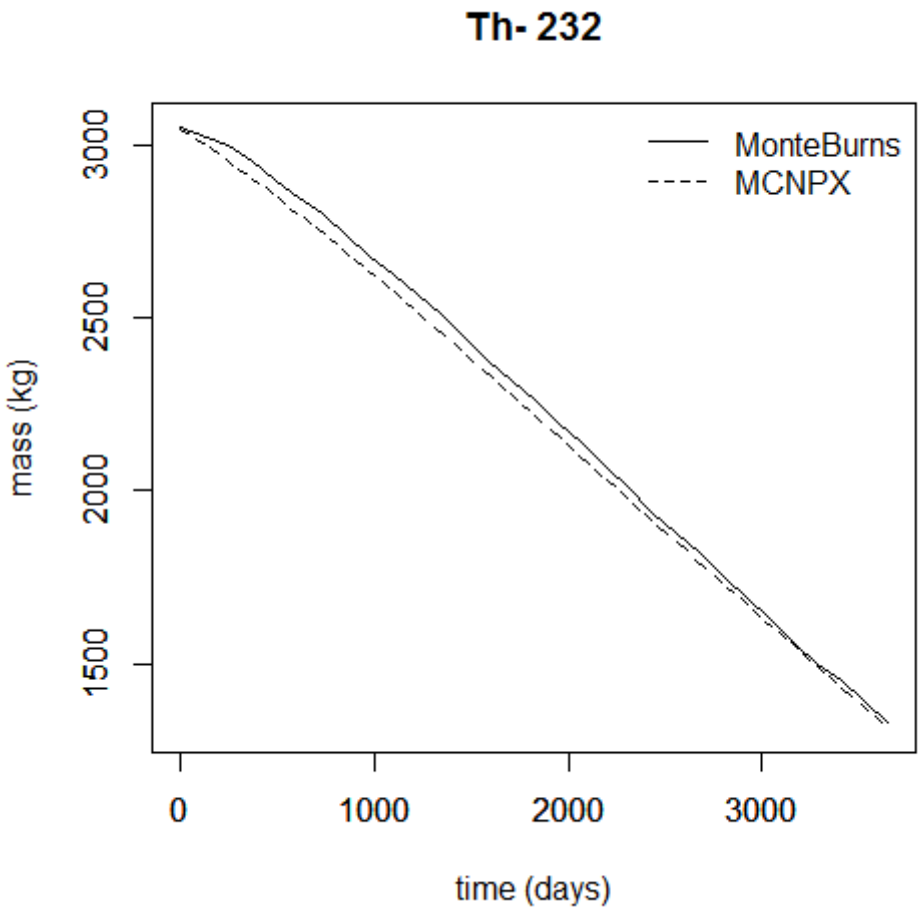

Figure 4: ^{232}Th mass variations.

Fig. 5 shows the ^{233}Pa concentrations during the 10 years of operation for the two codes. The ^{233}Pa production was very similar in the two simulations. It may be noted that this isotope is formed in small scale which contributes negatively to the reactivity. Furthermore, the protactinium effect is less severe for harder spectra like that. The protactinium effect is a relevant question in the neutron spectrum choice for a thorium fueled system. Protactinium captures neutrons (due to its large capture cross section) and, thus, decreases the reactivity and fuel regeneration. The capture cross-section for the ^{233}Pa in the fast region of the neutron spectrum is lower than in the thermal region, so the non-use of moderator facilitates the fuel regeneration by protactinium effect reduction.

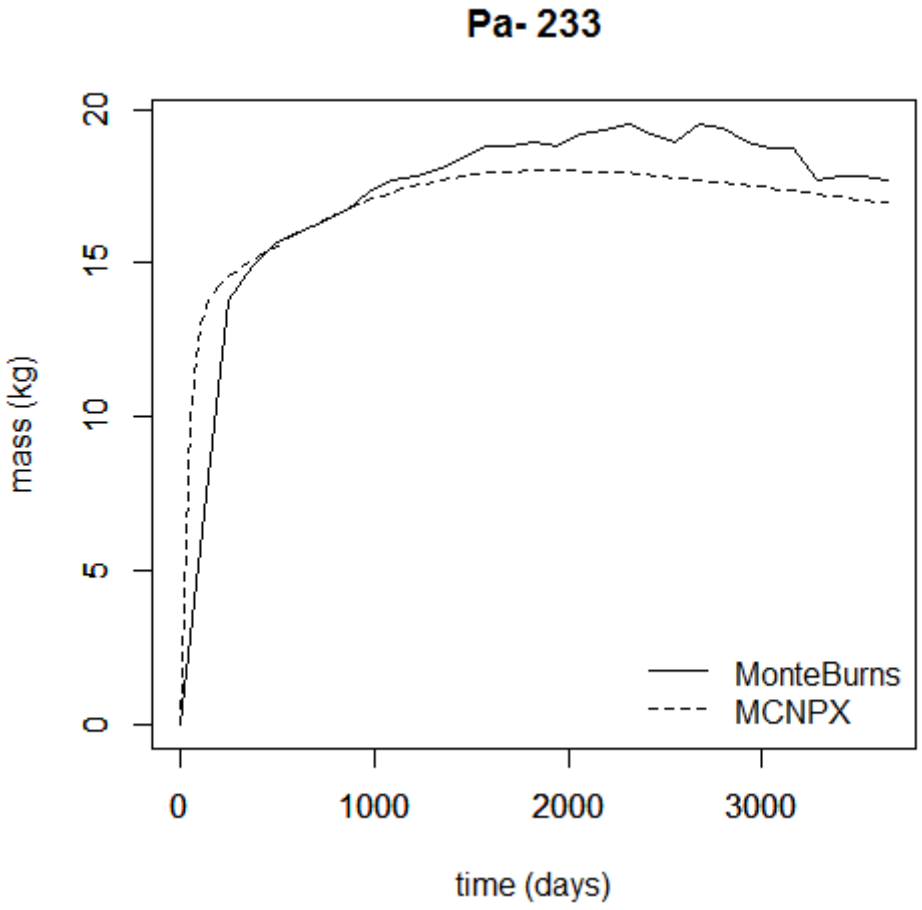

Figure 5: ^{233}Pa mass variations.

Fig. 6 presents the ^{233}U concentrations during the operation time. Once again there was a similar behavior in the isotope mass evolution. As can be verified in this figure the concentration of this isotope decreases with the time. This isotope is produced by the regeneration of the ^{232}Th, but it is constantly consumed for power generation, since the initial loading is used to generate 515 MW_t thermal power for 10 years. After all, the ^{233}U is the main fissile isotope of the system.

The burnup rate for the system simulated is 561.35 g/day. For ten years of operation the consumption is approximately 2049 kg of this isotope. It can be verified that the concentration of this isotope ^{232}Th is reduced by about 380 kg during the 10 years of operation for MCNPX simulation and about 365 kg for MONTEBURNS simulation. This indicates that not all the ^{233}U consumed for the power generation comes from initial loading system, but it comes from ^{232}Th regeneration.

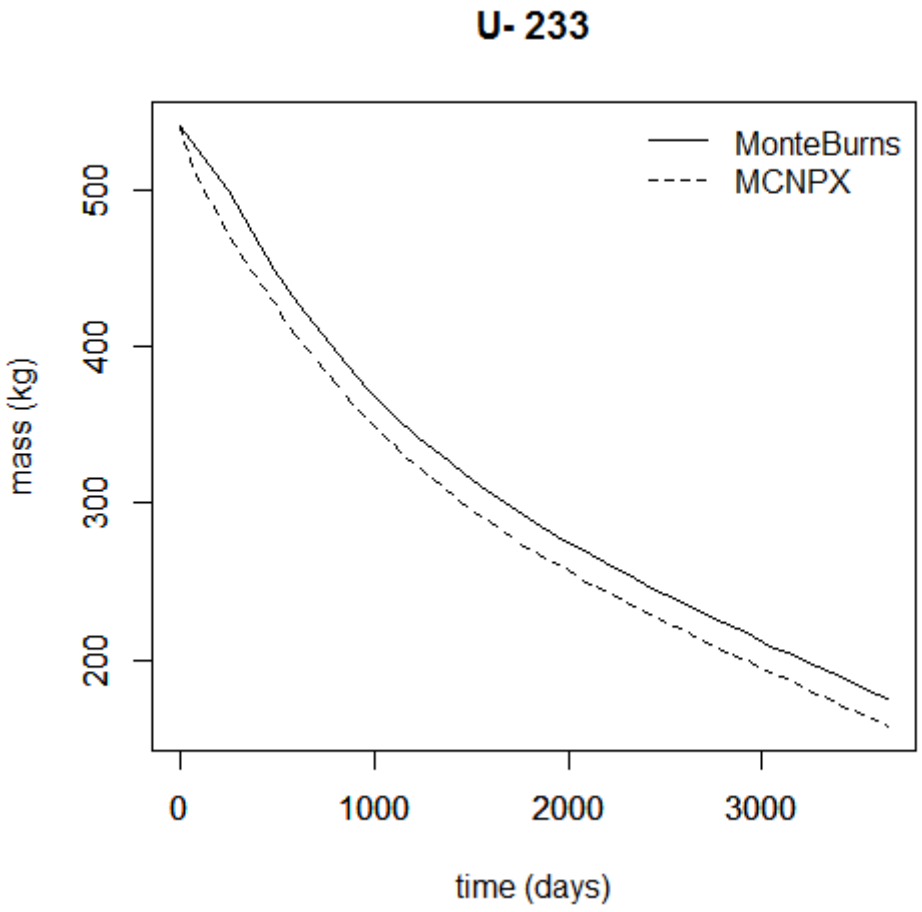

Figure 6: ^{233}U mass variations.

4. CONCLUSIONS

MONTEBURNS and MCNPX codes have proven to supply very similar results for an ADS simulation. Although the MCNPX code does not take into account the flux from external source during the burnup, the results of system criticality and the variation of the actinide inventory indicate a similar behavior between the results of both codes. Indicating that the MCNPX use for ADS simulations is a suitable choice for description of this systems evolution.

As future work will be simulated an ADS core fueled with thorium rods and burned fuel rods using MONTEBURNS. Such study was already performed using MCNPX [17]. Similarly, an ADS core fueled with thorium rods and reprocessed fuel rods previously performed using MCNPX [18], will be simulated using MONTEBURNS.

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