BURNUP SIMULATIONS OF DIFFERENT FUEL GRADES USING THE MCNPX MONTE CARLO CODE

by

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Scientific paper
DOI: 10.2298/NTRP1404259A

Global energy problems range from the increasing cost of fuel to the unequal distribution of energy resources and the potential climate change resulting from the burning of fossil fuels. A sustainable nuclear energy would augment the current world energy supply and serve as a reliable future energy source. This research focuses on Monte Carlo simulations of pressurized water reactor systems. Three different fuel grades – mixed oxide fuel (MOX), uranium oxide fuel (UOX), and commercially enriched uranium or uranium metal (CEU) – are used in this simulation and their impact on the effective multiplication factor (K_{eff}) and, hence, criticality and total radioactivity of the reactor core after fuel burnup analyzed. The effect of different clad materials on K_{eff} is also studied. Burnup calculation results indicate a buildup of plutonium isotopes in UOX and CEU, as opposed to a decline in plutonium radioisotopes for MOX fuel burnup time. For MOX fuel, a decrease of 31.9% of the fissile plutonium isotope is observed, while for UOX and CEU, fissile plutonium isotopes increased by 82.3% and 83.8%, respectively. K_{eff} results show zircaloy as a much more effective clad material in comparison to zirconium and stainless steel.

Key words: MCNPX code, burnup calculation, criticality calculation, radionuclide inventory

INTRODUCTION

Nuclear energy is a technologically mature and reliable source of base load power. It meets about 17% of the global demand for electricity [1]. In order for nuclear power to be sustainable in the long term, safe management practices which include better equipment design and operator safety guidelines, elimination and disposal of highly radioactive waste with minimum impact on the environment, as well as the implementation of better policies and disclosure of accurate information on matters relating to nuclear energy are neccessary in order to gain public trust.

Nuclear fuel burnup calculations give an important insight into the consumption and buildup of radionuclides during and after fuel fission in the nuclear reactor core. Fuel burnup is one of the crucial reactor core parameters in the operation of nuclear reactors [2]. During the process of fission in the reactor core, radionuclides are generated through the fission of a fissile or fissionable material, transmutation of a parent isotope or decay of a parent isotope to the isotope of interest [2]. Fuel burnup calculations are required for monitoring key reactor parameters such as reactivity and power distribution and also for the determination of fissile materials present at any moment during and after the fission process [3].

Radiological hazards emanating from severe reactor accidents can be accurately quantified from the knowledge of fuel burnup calculations [4]. The MCNPX code has the capability of simulating nuclear burnup reactions and calculating the radionuclide inventory due to fission of fissile or fissionable isotopes and the transmutation of parent nuclides. The code eliminates the need for the combination of the MCNP code with the nuclear burnup code Origen in which one group cross-sections and fluxes are transferred from MCNP to the decay code Origen using Monteburns [5].

The burning of nuclear fuel to generate energy in the nuclear reactor core gives rise to both short and long-lived radionuclides. Khattab *et al*. [4] estimated the total radioactivity of a miniature neutron source reactor (MNSR) using the GETERA code and highly enriched uranium as fuel. The total radioactivity of the

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MNSR was estimated based on a list of 19 identified radionuclides. This paper is aimed at analyzing the effect of different nuclear fuel grades on the radioactivity of the final fresh fission products after burnup in the reactor core. To do this, three different nuclear fuel grades – uranium oxide, mixed oxide fuels and commercially enriched uranium (uranium metal) – are utilized. Nuclear fuel burnup is carried out for 220 days with a 30-day time step and the total radio activities of radionuclides of the freshly burnt fuel analyzed at the end of the burn step. A number of factors determine the relative concentrations of radionuclides in a given fuel assembly, including the fuel material type, irradiation history and cooling time for a particular element [6]. Nuclear fuel clad material plays a key role in preventing radioactive fission products from escaping into the coolant. The clad material also conducts heat away from the fuel. The properties of a very good clad material are such that it must not only meet the chemical and mechanical limitations of the fuel design, but must also have an increased neutronic performance [7]. In this study, three different clad materials – zirconium, zircaloy, and stainless steel – are used to find out their effect on reactor core neutronic parameters such as K_{eff} and reactivity.

Table 1. Material composition of reactor core

Material name	Nuclide atom fractions
UO_2	^{16}O 5.85402E-3* ^{235}U 3.862438E-2 ^{238}U 9.555216E-1
Commercially enriched uranium	^{234}U 3E-4 ^{235}U 2.96E-2 ^{238}U 9.701E-1
Mixed oxide fuel	^{16}O 5.88402E-3 ^{235}U 2.5E-3 ^{238}U 9.386E-1 ^{238}Pu 1.1147E-4 ^{239}Pu 4.150E-2 ^{240}Pu 7.9657E-4 ^{241}Pu 1.001E-2 ^{242}Pu 5.6388E-4
Cladding (zirconium alloy)	Cr 9.98E-4 Fe 1.499E-3 Zr 0.982499 Sn 0.014999
Cladding (stainless steel)	Si 1E-1 Cr 0.17 Mn 0.02 Fe 6.55E-1 Ni 0.12 Mo 0.025
Moderator (light water)	^{1}H 4.7716E-2 ^{16}O 2.3858E-2 ^{10}B 3.6346E-6 ^{11}B 1.6226E-5

* E-3 means 10^{-3}

METHODOLOGY

Nuclear reactor core specification

The reactor core was modeled using the MCNPX visual editor. The core is made of a hexahedral lattice structure with light water as a moderator. The light water moderator, which also serves as a coolant, contains soluble boron-10 ions for the absorption of excess neutrons. The system geometry consists of a lattice arrangement of cylindrical fuel pellets entirely enclosed by a spherical surface. The average fuel and moderator temperatures are kept at 5400 K and 3000 K, respectively. The energy spectrum for neutron fluxes ranges between 1 MeV to 15 MeV, with the PWR capable of producing 950 MWe. The material composition of the reactor core showing nuclide atom fractions for the three fuel grades and also for the clad material and moderator used are shown in tab. 1.

The PWR model consists of a rectangular lattice design with cells belonging to three different universes. The radius of the fuel cylinder is 0.8 cm. The fuel lattice pitch is 2.5 cm. The inside and outside cladding diameters are 0.901 and 0.981 cm, respectively. The fuel grade assembly used consists of uranium oxide fuel with 3.86% enrichment of ^{235}U. The ^{235}U percent enrichment in commercially enriched uranium is 2.96% and 5.15% of fissile plutonium isotopes represented as ^{239}Pu and ^{241}Pu included into the mix for the MOX fuel.

MCNPX has the Cinder90 code integrated as a separate burnup module and should be more accurate than those simply linking the transport code and the Cinder90 code [8]. The MCNP input essentially consists of a number of data cards. Its geometry is based on four fundamental cards: a title card, cell cards, surface cards, and material data cards [9]. The title card begins the MCNP input and basically gives a label description for the other cards. The cell cards follow after the title cards and, essentially, indicate the connection between cells, surfaces and material data cards. The system geometry is expressed through a union or intersection of Boolean operators. The surface card gives surface numbers and the particular geometry of the surfaces. The last of the basic MCNP data cards is the material data card which gives material identification numbers and their compositions (atom or mass fractions). There are a number of data cards used by MCNP. These include the mode, the tally cards, the source specification cards, the material specification cards, *etc*.

A KSRC card is provided in the input data to run with the KCODE card in order to determine the criticality. The KSRC card typically sets the x, y, and z locations of fission (initial source points for fission). From the input data, the initial source point for fission is taken from the origin. In order to specify particular reaction types, $S(\alpha, \beta)$, thermal treatment cards are used. The atomic number (Z), mass number (A), and nuclide identification numbers (ID) for the thermal tables are taken directly from the evaluated nuclear data files (ENDF) and entered on an MTn card that is associated with an existing Mn card. A TMP card is used to indicate the temperature [K] at which the data were

processed. The TMP card parameters are 8.04E-8, 6E-8, 4.989E-8, and 8E-8 MeV. The temperature enters into the processing of the evaluation of a data file only through what is referred to as the Doppler broadening of cross-sections [9], a term used to describe the cross-section change resulting from the thermal motion of particles (in this case nuclei) in a target material. The thermal motion could be a result of translation, rotation, or vibration. The cinder.dat library file which contains the decay, fission yield and 63-group cross-section is utilized by MCNPX for burn-up calculations.

Rectangular lattice description

Two types of lattices are used for nuclear reactor core specifications – rectangular and hexagonal. The lattice structure may consist of several different shapes or identical shapes. A rectangular lattice for water-cooled reactors is used in this simulation. The lattice geometry is set up using the lattice fill matrix of the MCNPX visual editor. The rectangular lattice pitch is expressed in the axial x and y-directions as P_x and P_y. The number of unit cells in the x an y-direction, N_x and N_y gives the extent of the lattice structure. The total number of unit cells is hence N_xN_y [10]. The number of unit cells to the left and right of the center lattice element in the x- and y-direction is 24, as indicated by the fill card. The lattice cell structure is shown in fig. 1. This is a simplified model of a rectangular lattice with five unit cells for its specification. The lattice cell card used is

```
3 0 8   7 10   9   u   1 lat   1
   fill    24:24   24:24   0:0
```

The first number is the cell number, which is 3. The second number is the material number and is 0, indicating a void material. Unless the fill entry in the fill matrix is the same as the universe number of the lattice, the material number is often ignored when setting up the lattice structure [11]. The next four numbers are the surface numbers for the planes, which are sides of the rectangular shape. The U card specifies the universe to which the cell belongs, which in this case is 1. A cell is filled with a universe, which is either a lattice or an arbitrary collection of cells. The lat card specifies the particular kind of lattice, which is 1 for a rectangular lattice and 2 for a hexagonal lattice. The fill card specifies the universe, which fills a particular cell. The system geometry as modeled by the MCNP visual editor is as shown in fig. 2 .The geometry shows the coolant water together with the fuel pins and the unit cell lattice.

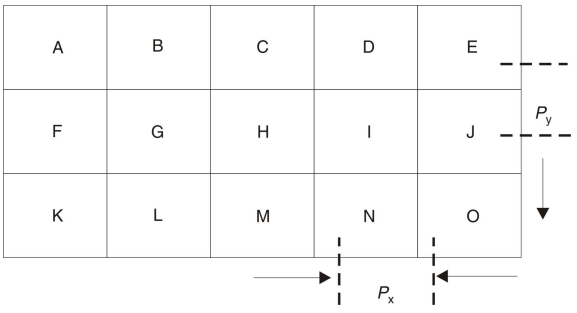

Figure 1. Rectangular lattice with five parameters for its specification

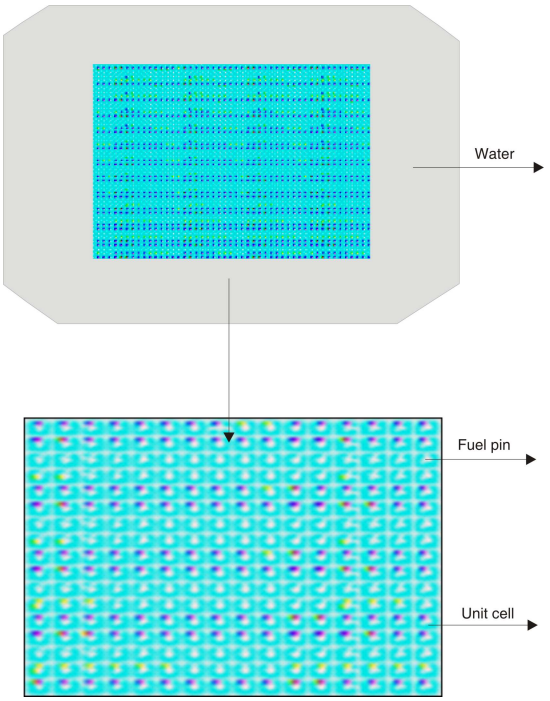

Figure 2. MCNPX simplified model of reactor core assembly

RESULTS AND DISCUSSION

Choice of material for cladding

The material used for the cladding prevents the nuclear fuel from making direct contact with the coolant inside the reactor vessel. This is to prevent the potential for radioactivity to be released into the reactor core environment. The choice of material for the cladding should meet the following requirements:

– it should not absorb neutrons which could be used to initiate further fission reactions, and
– it should have a high thermal conductivity, but not a high thermal expansion coefficient

As indicated above, a good cladding material must have a low thermal absorption cross-section for neutrons, as well as high thermal conductivity. The high thermal conductivity is to enable effective heat transfer from the fuel rod to the coolant in order to prevent excessive temperature buildud leading to the melting of the fuel material. The neutron absorption cross-section,

Table 2. Neutron absorption cross-sections and thermal conductivities for common clad materials at 25 °C [11]

	Cr	Si	Mn	Fe	Ni	Mo	B	Sn	Zr	Zr-alloy	Steel
σ_a [b*]	3.1	0.17	13.3	2.56	4.49	2.6	750	0.63	0.184	0.22	3.1
k [$Wm^{-1}K^{-1}$]	93.9	149.2	7.81	79.5	90.9	138	27.4	66.8	22.6	21.5	16

*1 b = 10^{-28} m^2

Table 3. K_{eff} values for different clad materials at the beginning (BOL) and end (EOL) of burnup steps using MOX fuel

FUEL	CLAD	K_{eff} at BOL		K_{eff} at EOL	
MOX	Stainless steel	1.09295	0.00138	0.92315	0.00087
MOX	Zircaloy	1.15778	0.00145	0.98630	0.00098
MOX	Zirconium	1.15624	0.00151	0.98258	0.00098

Table 4. K_{eff} values for different clad materials at the beginning (BOL) and end (EOL) of burnup steps using UOX fuel

FUEL	CLAD	K_{eff} at BOL		K_{eff} at EOL	
UOX	Stainless steel	0.90130	0.00193	0.81205	0.00212
UOX	Zircaloy	0.95456	0.00140	0.80834	0.00077
UOX	Zirconium	0.93740	0.00236	0.80754	0.00049

Table 5. K_{eff} values for different clad materials at the beginning (BOL) and end (EOL) of burnup steps using CEU fuel

FUEL	CLAD	K_{eff} at BOL		K_{eff} at EOL	
CEU	Stainless steel	0.91187	0.00311	0.80920	0.00097
CEU	Zircaloy	0.97923	0.00210	0.86789	0.00105
CEU	Zirconium	0.95529	0.00232	0.84828	0.00054

σ_a, is a parameter which measures the neutron absorption potential of the substance. Its unit is in barn, a unit of area equal to 10^{-28} square meters. Table 2 shows the thermal neutron absorption cross-sections of some common clad materials at 20 °C thermal incident neutrons and thermal conductivities at 25 °C.

Tables 3-5 show the K_{eff} results of the different clad materials when used with MOX, UOX, and CEU fuel, respectively. From the neutron absorption cross--section in tab. 3, the thermal neutron absorption of zirconium and zircaloy is much lower than that of stainless steel. This explains the good K_{eff} value obtained for zircaloy and zirconium clad materials as compared to steel. The absorptivity also explains the degree of neutron interaction with the clad material. For zirconium and zircaloy, not many neutrons are absorbed and, hence, these neutrons remain in the reactor core and are able to initiate further fission processes. This also makes zirconium very effective in preventing radioactive fission fragments from escaping the fuel into the coolant and contaminating it. Again, when UOX and CEU fuel grade materials were used as shown in tabs. 4 and 5, similar patterns of K_{eff} were obtained with zirconium and zircaloy, showing much better results for the K_{eff} as compared to stainless steel. Even though zirconium has a slightly lower neutron absorption cross-section and comparable thermal conductivity relative to the zirconium alloy, as shown in tab. 2, K_{eff} results for zircaloy are slightly higher than those for zirconium. This observation may be due to enhanced alloy properties.

The zircaloy cladding used is zircaloy-4, which is similar in composition to zircaloy-2, but has reduced nickel and iron compositions. The reaction of zirconium with steam at high temperatures produces hydrogen gas by the reaction:

$$Zr + 2H_2O \quad ZrO_2 + 2H_2$$

This reaction leads to zirconium metal oxidation. It reduces the ductility and robustness of the zirconium metal and hence increases the probability for the escape of thermal neutrons from the core of the reactor. It also reduces the effectiveness of zirconium for higher and prolonged fuel burnup. For zirconium alloys, the hydrogen produced by the oxidation of zirconium in steam diffuses into the alloy, causing the formation of zirconium hydrides. The hydrides formed are less dense and more brittle than the zirconium alloy, leading to the weakening of the clad material. This is the case especially with the zirconium-2 alloy. The zirconium-4 alloy used has reduced composition of iron and no nickel composition. This reduces the hydride effect by reducing the tendency to pick up hydrogen. The said characteristic of zircaloy-4 improves its mechanical properties, lessening the probability of escape of thermal neutrons and thus improving the overall K_{eff} value in the long term.

A look at thermal conductivities in tab. 2 also reveals a higher value for zirconium and zircaloy, as compared to that of stainless steel. This helps in conducting the heat away from the reactor core to the coolant quickly, a property which prevents very high temperature buildup in the core leading to the melting of the fuel material or clad. The thermal conductivity of zirconium alloys is superior to that of stainless steel. This property makes zirconium alloys much more stable at very high temperatures. Thus, zircaloy is recommended as an effective clad material.

Burnup calculations

As the burning of the nuclear fuel proceeds in the reactor, the fission of fissile and fissionable isotopes,

as well as the transmutation of parent nuclides, leads to the inventory of various kinds of nuclides. Some of these nuclides are transuranic elements, while others are fission products. The buildup of some of these fission products (actinides) constitutes poison in the nuclear fuel reactor and reduces the reactivity and power distribution (*e. g.* ^{135}Xe). Again, the depletion of some isotopes such as ^{235}U reduces reactivity. Burnup also helps determine the lifetime of the reactor core which is the length of reactor operating time at which the effective multiplication factor remains 1. This is done by studying the time evolution of K_{eff}. The pattern of the variation of the radionuclide inventory with time can be studied from burnup results. Finally, the total radioactivity of the reactor core can be determined by summing up the radio activities of all important nuclides after core life so as to determine the extent of the radiological hazard posed in the event of exposure to the environment. The fuel material grades were burned for a period of 220 days at 30 days time steps, using zircaloy as clad material. A 10 day cooling period is allowed after the second time step and there is no fuel burnup. However, during this cooling period, the fuel material may decay slightly.

The variation of actinides and some key non-actinides with burnup time is analyzed. In all, the uranium nuclide inventory shows similar variation with burnup time for all three different fuel grades. In figs. 3(a) and 3(c), there is a decrease of ^{235}U and a slightly lower decrease for ^{238}U with burnup time because these radionuclides are consumed as the fission process progresses. In fig. 3(b), ^{236}U radioisotopes, which are not fissile with thermal neutrons and are generated mainly due to the gamma radiation emission of ^{235}U as fission proceeds, are observed to increase with burnup time for each of the three fuel grades. Very little of ^{238}U is consumed in the fission process as it is only fissionable and the main fissile material is ^{235}U which decreases rapidly. The uranium inventory is found to decrease for MOX fuel, but on a slightly lower scale relative to other fuel grades, due to a relatively small uranium composition used in its fabrication.

For the fissile plutonium isotope inventory, there is a substantial decrease in fissile isotopes of ^{239}Pu and ^{241}Pu for the MOX fuel fig. 4(a) and fig. 4(c) as plutonium forms the main fissile composition of MOX fuel. However, an increase in fissile plutonium isotopes with burnup time is observed for UOX and CEU. This is primarily due to the formation of heavier isotopes as the fission process proceeds, mainly due to neutron capture by ^{238}U. This plays a major role in the reduction of radio hazard due to fissile plutonium isotopes. For instance, for MOX fuel, there is an observed decrease of 31.9% of fissile plutonium isotopes after fuel burnup, while the fissile plutonium isotope increased by 82.8% in UOX fuel and showed an 83.9% increase in CEU fuel. In fig. 4(b), the ^{240}Pu isotope is observed

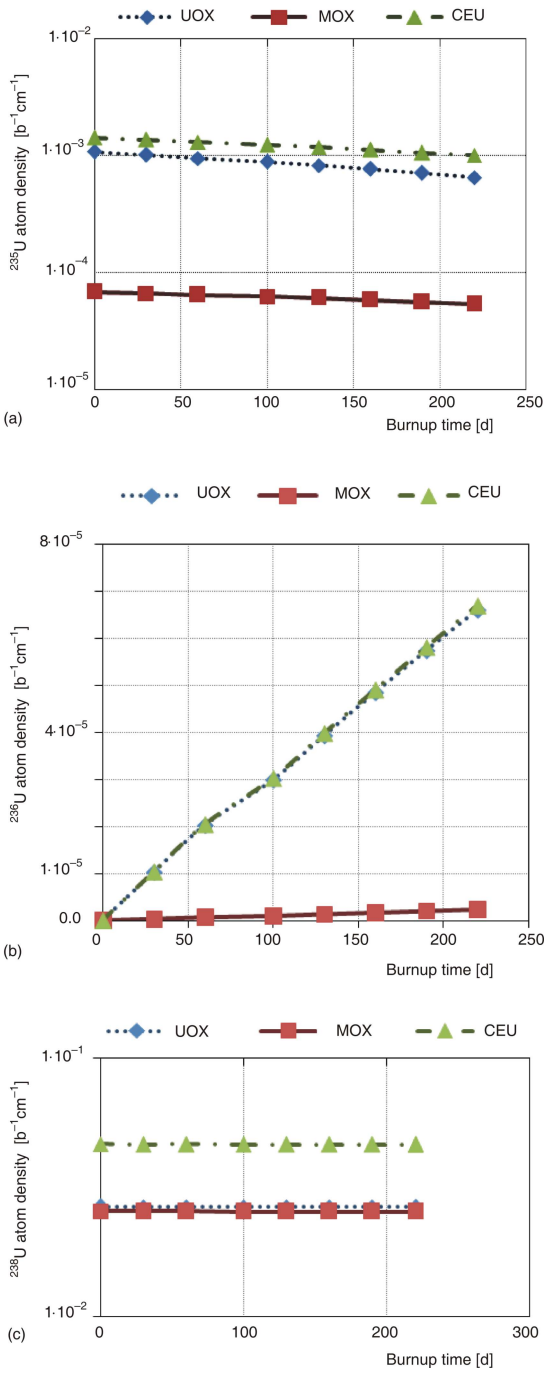

Figure 3. Atom density *vs.* burnup time for (a) ^{235}U, (b) ^{236}U, and (c) ^{238}U

to build up steadily for each of the three fuel grades. The ^{240}Pu radioisotope, however, rises on a much higher scale in MOX than in CEU and UOX. This is because ^{240}Pu is formed in the nuclear reactor by occasional neutron capture by ^{239}Pu, much of which forms the initial fissile fuel material in MOX fuel. The concentration of ^{240}Pu builds up steadily since it is not fissile and, hence, does not undergo fission to produce energy.

For ^{135}Xe in fig. 5(a), a similar pattern is observed for all three fuel grades. There is a rapid accumulation of ^{135}Xe after the first burn step, a result that

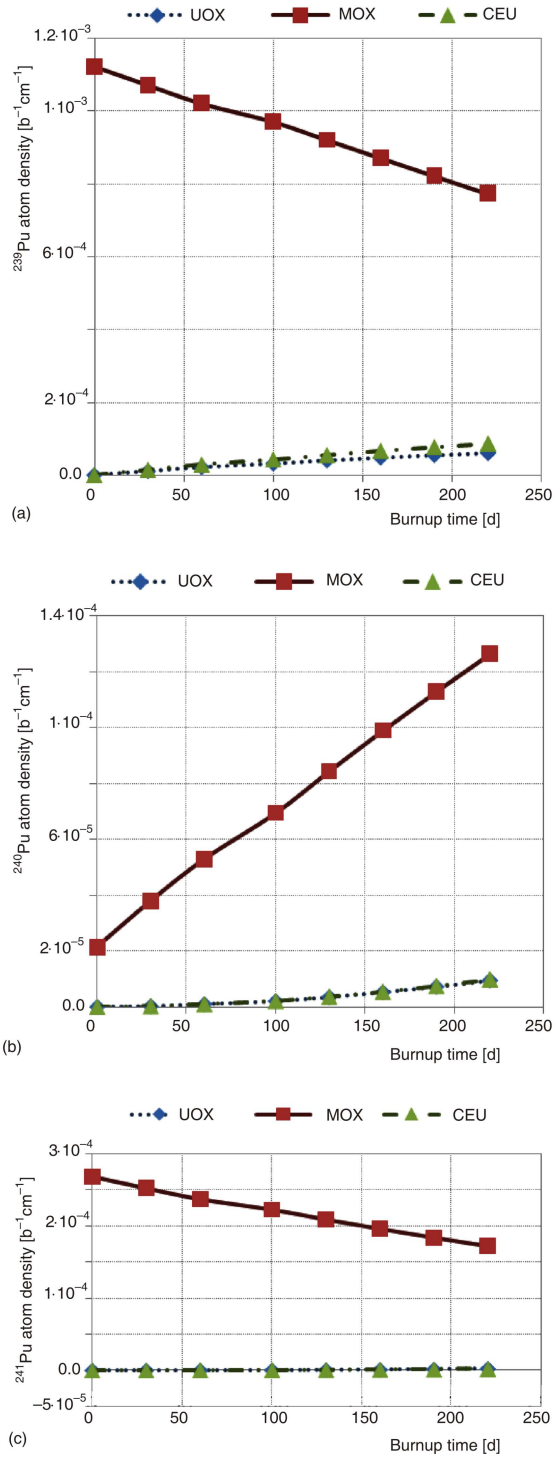

Figure 4. Atom density *vs.* burnup time for (a) ^{239}Pu, (b) ^{240}Pu, and (c) ^{241}Pu

might lead to a drastic drop in K_{eff}. This is known as *xenon poisoning*. The production of ^{135}Xe isotopes after this burn step gradually slows down, a result which helps regulate the reactivity of the system. The accumulation of the fission product ^{134}Cs fig. 5(b) shows a linear variation with burnup time for all three fuel grades.

The pattern of the variation of burnup with time for the three fuel grades shows a substantial decrease

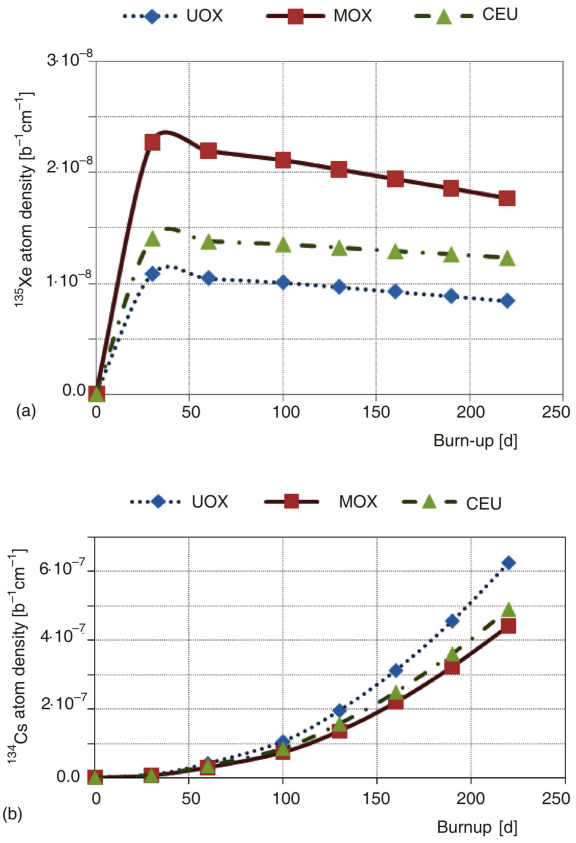

Figure 5. Atom density *vs.* burnup time for (a) ^{135}Xe and (b) ^{134}Cs

in ^{239}Pu and ^{241}Pu for MOX, but an observed increase in these fissile isotopes for UOX and CEU. The half-life of ^{239}Pu is 24100 years and that of ^{241}Pu is 14.4 years. The decrease of these isotopes during fuel burnup for MOX essentially reduces the radioactivity of the final product after burnup. MOX fuel also has a smaller uranium isotope fraction (^{235}U and ^{238}U) relative to UOX and CEU. Uranium isotopes have half-lives of several millions of years and thus its smaller fraction in MOX fuel further reduces the radioactivity after core burnup.

Nuclear fuel reactivity and effective multiplication factor

Reactivity is the degree of neutron multiplication in the reactor core. The higher the excess reactivity, the larger the energy output for a particular fuel. Factors which affect reactivity include the density and temperature of the coolant and also the fuel temperature and density.

The reactivity for the three different fuel grades is calculated as a function of burnup and peak reactivity determined for each fuel grade. Peak reactivity is the highest reactivity obtained as a function of burnup for each fuel grade. One of the most important measures of fuel performance is peak reactivity. Since re-

Table 6. Peak reactivity parameters for the different fuel grades

Reactivity ρ	UOX	MOX	CEU
Peak	0.181	0.174	0.128

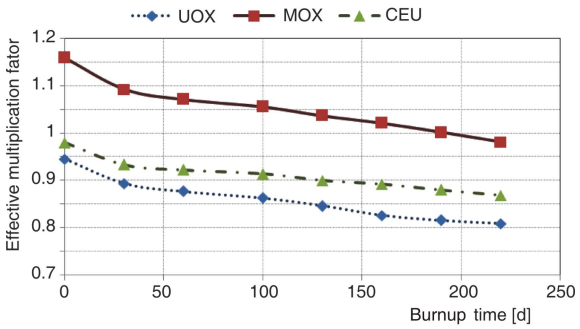

Figure 6. Comparison of K_{eff} *vs.* burnup time for different fuelgrades

activity has a direct bearing on the power level, the higher the peak reactivity, the higher the power output. Peak reactivities of the three different fuel grades as burnup proceeds are presented in tab. 6.

A look at the compositions of the three fuel grades reveals that ^{235}U forms the main fissile material in both UOX and CEU. The depletion of ^{235}U is known to reduce reactivity. The buildup of actinides due to neutron absorption of ^{238}U is also known to reduce reactivity. These two factors occur in both UOX and CEU and might cause loss of reactivity, but this is compensated by the buildup of ^{239}Pu and ^{241}Pu for these two fuels. In MOX fuel, the depletion of ^{235}U and ^{238}U reduces reactivity. However, the reactivity for MOX fuel is further reduced by the depletion of ^{239}Pu and ^{241}Pu which are the main fissile material in MOX fuel. This is seen in the low peak value recorded for MOX fuel relative to that of UOX fuel, as shown in tab. 6.

The study of the variation of K_{eff} with core burnup is of great importance as it describes whether or not the chain reaction in a nuclear reactor is stable or self-sustained. The results also give important details on core lifetime, defined as the length of time the reactor's effective multiplication factor is above one [13]. There is a large drop in K_{eff} during the first burn step, as shown in fig. 6. This drop can be attributed to a drastic reduction in reactivity due primarily to the buildup of burnable poisons such as ^{135}Xe and the depletion of fresh fuel. The K_{eff} is then gradually seen to decrease with time in subsequent burn steps. A similar pattern of the variation of K_{eff} with time is observed for all three different fuel grades. MOX fuel, however, might be especially effective in improving the core lifetime of the reactor as K_{eff} is observed to remain critical for a much longer time relative to other fuels. For UOX and CEU to maintain criticality for a longer burn time, an

Table 7. Total activities of actinides and non-actinides for the three fuel grades after core burnup

Fuel	Actinide activity [Bq]	Non-actinide activity [Bq]	Total activity [Bq]
UOX	1.65E+19*	2.60E+19	4.25E+19
MOX	1.05E+19	2.59E+19	3.64E+19
CEU	1.94E+19	2.62E+19	4.57E+19

*1.65E+19 means 1.65 10^{19}

increase in the mass fractions or weight percent (particularly for fissile isotopes) is required. This is not too desirable, due to the extremely high cost involved.

Cuvelier and Tsvetkov[13] showed that transuranic fuels (TRU) extend the core lifetime of a reactor by about 36% when a part of low enriched uranium (LEU) was replaced by TRU in a miniature neutron source reactor. This shows the ability of the transuranic fuel to remain critical for a much longer time.

Atom densities and radio activities, in Bq, were calculated for each of the three fuel grades at the end of a 220 day burnup. Total radio activities of both actinides and non-actinides were calculated for each fuel grade and presented in tab. 7. Total atom densities and radio activities are very important parameters in estimating which fuel grade performs better, thus posing a relatively lesser hazard at the end of the burnup time or core lifetime of the reactor. For the same burnup time, MOX fuel is found to have a relatively lesser total radioactivity of the reactor core, almost a 15% reduction in comparison to other fuel grades.

CONCLUSIONS

Nuclear fuel burnup calculations give an important insight into the consumption and buildup of radionuclides during and after fuel fission in the nuclear reactor core. In this research, a Monte Carlo burnup simulation of a critical pressurized water reactor system is carried out using three different fuel grades (UOX, MOX, CEU) and the effect of different clad materials (zirconium, zircaloy, and stainless steel) on the K_{eff} is also analyzed.

Zircaloy, with a low thermal neutron absorption cross-section and high thermal conductivity has produced better results for K_{eff} and, hence, proves to be a much more effective clad material. The percent difference of K_{eff} for zircaloy relative to zirconium and stainless steel was found to be 2% and 8%, respectively, for all three fuel grades.

The atom densities and radio activities, in Bq, were calculated for each of the three fuel grades at the end of a 220 day burnup. Total atom densities and radio activities of both actinides and non-actinides were calculated for each fuel grade. This was found to be 4.251 10^{19} Bq for UOX fuel, 3.639 10^{19} Bq and 4.567 10^{19} Bq for MOX and CEU fuel, respectively. Total atom densities and radio activities are very im-

portant parameters in estimating which fuel grade performs better in the sense of posing relatively fewer hazards at the end of the burnup time or core lifetime of the reactor. There was an observed decrease of 31.9% of fissile plutonium isotopes for MOX fuel, whilst the fissile plutonium isotope composition increased by 82.8% and 83.9% for UOX fuel and CEU fuel, respectively. For the same burnup time, MOX fuel was found to have a relatively less total radioactivity of the reactor core, almost a 15% reduction, as compared to the other fuel grades.

ACKNOWLEDGEMENT

This work is supported by a grant from the National Science Foundation (NSF) through the Center for Energy and Environmental Sustainability (CEES) NSF CREST Center. Award # 1036593.

AUTHOR CONTRIBUTIONS

MCNPX simulations and data processing were done by F. Asah-Opoku under the supervision of Z. Liang and R. R. Kommalapati. Discussions regarding this paper were held with R. R. Kommalapati and Z. Huque. The writing of the manuscript, including figures and tables, were done by F. Asah-Opoku.

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Received on August 26, 2014
Accepted on October 6, 2014

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СИМУЛАЦИЈЕ ИЗГАРАЊА РАЗЛИЧИТИХ ВРСТА ГОРИВА УПОТРЕБОМ MCNPX МОНТЕ КАРЛО ПРОГРАМА

Глобални енергетски проблеми распростиру се од пораста цене горива до неравномерне расподеле енергетских извора и могуће промене климе услед сагоревања фосилних горива. Одржива нуклеарна енергија могла би да повећа садашње снабдевање света енергијом и да послужи као поуздан енергетски извор у будућности. Овде приказано истраживање усмерено је на Монте Карло симулације реакторских система са водом под притиском. Три различите врсте горива – мешано оксидно гориво (MOX), уранијумоксидно гориво (UOX) и комерцијално обогаћен уранијум или уранијум метал (CEU) – коришћена су у симулацијама и анализиран је њихов утицај на ефективни фактор умножавања K_{eff} и, отуда, критичност и укупну радиоактивност реакторског језгра по изгарању. Такође је размотрен утицај различитих материјала кошуљица горива на K_{eff}. Резултати прорачуна изгарања указују на уградњу изотопа плутонијума у UOX и CEU горивима, насупрот смањењу радиоизотопа плутонијума у MOX гориву у току изгарања. За MOX гориво утврђено је смањење од 31.9% у фисибилним изотопима плутонијума, док се за UOX и CEU горива фисибилни изотопи плутонијума увећавају за 82.3% и 83.8%, респективно. Резултати за K_{eff} показују да је циркалој много делотворнији материјал за кошуљицу у односу на цирконијум и нерђајући челик.

Кључне речи: MCNPX програм, прорачун изгарања, прорачун критичности, инвентар радионуклида