Proceedings of the HTR 2012
Tokyo, Japan, October 28 – November 1, 2012
Paper HTR2012-5-002

Fuel Pebble Design Studies of a High Temperature Reactor using Thorium

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Abstract – *In this paper the optimal design, in terms of thorium to U-233 conversion, of a fuel pebble in a pebble bed High Temperature Reactor (HTR) using thorium is investigated. Using SCALE6 the infinite multiplication factor and nuclide concentrations are calculated during depletion. Pebbles with thorium and different initial U-233 weight fractions are studied for heavy metal loadings up to 30 g, a conservative estimate for fuel fabrication. Middle-of-life burnup pebble cross sections are used as a surrounding material in the depletion calculation scheme to provide a more realistic neutron spectrum. The influence of this will be presented in the paper.*

Using larger, instead of more, fuel kernels only leads to a small increase of the multiplication factor. Fuel lumping does on the other hand lead to a significant decrease of the thorium to U-233 conversion. Lower specific powers result in higher multiplication factors during burnup, while the U-233 concentration hardly changes. The conversion of thorium into U-233 can be maximized for thorium pebbles with a large heavy metal loading of 30 g, using the standard fuel kernel radius of 0.025 cm, irradiated at low specific power. Without fuel reprocessing, the addition of moderator pebbles is required to raise the infinite multiplication factor of these pebbles above one. For core design studies it is recommended to insert fresh pebbles with 30 g thorium into one or multiple breed zones, without moderator pebbles, while the irradiated pebbles are recycled into one or multiple driver zones with moderator pebbles.

Reactivity coefficients of Th/U-233 fuelled pebbles have also been determined. Though the moderator temperature feedback is generally positive the uniform temperature coefficient is negative for the 30 g heavy metal pebble. Only a limited number of moderator pebbles may be added to maintain a negative uniform temperature coefficient.

I. INTRODUCTION

Pebble bed reactors are designed with a negative temperature feedback and a pathway for decay heat removal by means of passive cooling. The design ensures that the fuel temperature inside the core never exceeds 1600 °C. The thousands of graphite pebbles inside a PBR contain many small fuel kernels surrounded with protective TRISO layers, which retain all fission products within the fuel particle for temperatures up to 1600 °C. These inherently safe characteristics give high temperature reactors a significant advantage over other current reactor designs. Other advantages of the pebble bed reactor can be found in the capability of online refueling, its possibility to achieve high fuel burnups and the high temperature of the heat produced in the core. The high outlet temperatures allow for efficient electricity production, but also offer opportunities for industrial applications and hydrogen production.

For future energy supply it is very interesting to investigate the combination of the inherent safety and high temperature applications of the pebble bed reactor design and the usage of thorium as a nuclear fuel. The thorium fuel cycle has several interesting advantages. Thorium is three to four times more abundant in the earth's crust than uranium. The use of thorium can reduce the radiotoxicity and required storage time of the nuclear waste. The $^{233}U/^{232}Th$ fuel cycle has favourable nuclear properties for use in thermal breeder reactors, as compared to the ^{238}U/Pu-cycle. Furthermore, ThO_2-fuels are chemically more stable, have a higher radiation resistance and favourable thermophysical properties over UO_2-based fuels. ThO_2 is also relatively inert making the long term storage and permanent disposal of spent fuel simpler as oxidation is no problem. The inertness can on the other hand complicate the fuel fabrication.[1][2]

Thorium is not a fissile isotope by itself. It has to be converted in a nuclear reactor into U-233. Neutron capture inside Th-232 leads to the formation of Th-233 ($t_{1/2}$=22.3 m), which forms Pa-233 via β-decay. Secondly Pa-233 ($t_{1/2}$=26.967 d) via β-decay forms the fissile isotope U-233. Very relevant for the neutronics is that Pa-233 is a strong neutron absorber. If a neutron is captured in Pa-233 not only a neutron is lost but also a potential fissile atom, as it cannot decay to U-233 anymore.

The neutron capture cross section for thermal neutrons in Th-232 is 7.4 barns compared to 2.7 barns for U-238 leading to higher fertile to fissile conversion ratios for Th-232. Secondly, the number of neutrons produced per neutron absorbed in U-233 is greater than 2.0 over a wide energy range of the thermal neutron spectrum. Unlike the ^{238}U/Pu-cycle, the Th/^{233}U-fuel cycle can therefore also achieve breeding for thermal neutron spectra. [2][3]

The use of thorium inside the pebble bed reactor has been investigated on paper and in practice in the past in order to reduce uranium resource usage and to reduce the amount of higher actinides produced in or fed to the reactor, especially in combination with plutonium. [4][5]

The use of thorium for the incineration of plutonium inside HTRs, as a means of reducing the large stockpiles of plutonium worldwide, has been investigated by both Rütten and Haas [4] and Chang et al. [5] on the basis of the HTR-MODUL design. Burning plutonium in combination with thorium produces only negligible amounts of second-generation plutonium [4] and a large fraction of the plutonium could be depleted [5].

Thorium fuel was also used in practice in the Thorium High Temperature Reactor (THTR, 300 MWe), which reached its first criticality in September 1983. The pebble bed consisted of 675000 pebbles and the cylindrical core was 5.6 m in diameter and around 6 m high. A THTR fuel element contained 0.96 g of highly enriched U-235 and 10.2 g of Th-232. On average a pebble would make six passes through the core up till a final burnup of around 110000 MWd/t_{hm}. The THTR was shut down in August 1989 for economic reasons, as the different participants could not agree on how to cover the financial risks during the operation and decommissioning of the THTR. [6]

More interesting for the present work is the research related to pebble bed reactor designs with a high conversion ratio (> 0.9). In the seventies Teuchert and Rütten [7] investigated thorium based fuel cycles in the pebble bed reactor with the conversion of thorium into U-233 as the main interest. Teuchert and Rütten investigated pebble bed reactors with a maximum discharge rate of U-233 (CR=0.76) and a near breeder pebble bed reactor (CR=0.97). The first reactor type can be used to supply the make-up fuel of over 10 near breeder pebble bed reactors. The average conversion ratio of this combined system is mentioned to be 0.95. The design and operation of the two reactor types are identical. This allows to alternate between the near breeder and maximum discharge design during full power operation. Teuchert and Rütten [7] also state that it is possible to raise the conversion ratio of the reactor concept above one with a rigorous reduction of parasitic losses of neutrons.

In another paper from 1975 Teuchert and Rütten also investigated several fuel cycles in the pebble bed reactor, among which the recycling variant of the thorium fuel cycle [8]. According to Teuchert and Rütten a conversion ratio in the range of 0.9 and 1.0 can be reached. In their calculations a conversion ratio of 0.958 was found by a minimization of the average burnup to 24000 MWd/t_{hm}, a reduced power density and an increase of the heavy metal loading to 33 grams per pebble.

Less research on thorium PBRs with a high conversion ratio has been reported in recent years. The design of an inherently safe thorium breeder pebble bed reactor would be a major achievement in terms of safety and sustainability. This involves optimization studies of fuel and core design to optimize the conversion ratio. Calculations of thermal-hydraulics and reactivity coefficients are also required for the safety analysis. Furthermore the operating conditions of the thorium fuelled PBR should be feasible from a practical and economical point of view.

Before optimizing the neutronics of the thorium pebble bed core design, an optimization study of the fuel design needs to be performed. The results of this study are presented in this paper.

For the fuel design studies, the influence of several parameters on the multiplication factor of a single fuel pebble in an infinite lattice was studied, both for fresh Th/^{233}U fueled pebbles and during burnup. For the fresh fuel pebbles, the influence of the number of TRISO particles per pebble, the fuel kernel radius and the U-233 weight fraction upon the infinite multiplication factor has been investigated, as well as the influence of using a mixture of fuel and moderator pebbles. The fresh fuel pebble calculations and results are presented in section II.

The influence of the number of TRISO particles per pebble, the fuel kernel radius and the initial ^{233}U weight fraction on k_{inf} and the nuclide concentrations have been investigated as a function of burnup. The effect of the magnitude of the specific power on k_{inf} during fuel depletion has been investigated for a pebble with a high heavy metal loading. In the depletion calculation scheme, middle-of-life burnup pebble cross sections are used as a surrounding material to provide a more realistic fuel kernel spectrum. The calculational method and the results for the parametric studies of the fuel pebble depletion are presented in section III. Thorium pebble reactivity coefficients are discussed in section IV followed by the conclusions in section V.

II. FRESH FUEL PEBBLE PARAMETER STUDIES

Fuel pebbles consist of several thousands of TRISO coated fuel particles dispersed in a graphite matrix surrounded by a fuel free graphite shell. Each coated fuel particle consists of a fuel kernel surrounded by a porous carbon layer, an inner-pyrolitic carbon layer, a silicon-carbide layer and an outer-pyrolitic carbon layer. Possible variations in the fuel design are the fuel kernel size, the number of fuel particles and graphite matrix diameter.

Table 1: Pebble nuclide concentrations in atoms/(barn·cm)

Fuel design layer	**Nuclide**	**Atom density**
Carbon buffer	C	$5.2645 \cdot 10^{-2}$
Inner PyC layer	C	$9.5262 \cdot 10^{-2}$
SiC layer	C	$4.7760 \cdot 10^{-2}$
	Si	$4.7760 \cdot 10^{-2}$
Outer PyC layer	C	$9.5262 \cdot 10^{-2}$
Graphite matrix	C	$8.7741 \cdot 10^{-2}$
Pebble outer shell	C	$8.7741 \cdot 10^{-2}$
Coolant	He	$5.5740 \cdot 10^{-4}$

The nuclide concentrations in table 1 were used during the calculations for the TRISO buffer layers and the pebble coating layers [9]. For most of the calculations a pebble temperature of 1300 K was used.

For the calculations the geometrical properties in table 2 are used for the coating layers and the pebble. A variation of the fuel kernel radius might require a change of the TRISO coating layer thicknesses to ensure the retention of all the fission products. It is however not evident whether a simple (linear) relation exists between the fuel kernel radius and the desirable coating thicknesses. The thickness of the coating layers has an almost negligible influence upon the neutronics. Hence constant TRISO coating layer thicknesses are used in all of the calculations. For the fuel inside the kernel a mixture of UO_2 and ThO_2 is used, where for uranium the U-233 isotope is meant.

Table 2: Geometric properties of fuel pebble and TRISO coatings

Geometric property	
C-buffer layer thickness	0.09 mm
Inner PyC-layer thickness	0.04 mm
SiC layer thickness	0.035 mm
Outer PyC layer thickness	0.035 mm
Fuel zone radius	2.5 cm
Pebble outer diameter	3.0 cm
Pebble packing fraction	0.61

The unit cell calculations of the fresh fuel pebble are performed using the CSASI sequence of the SCALE6 code package. The DOUBLEHET-module is used inside the CSASI sequence to include the double-heterogeneity of the fuel into the calculation. The DOUBLEHET module uses CENTRM/PMC to perform the resolved resonance processing for multi-group cross sections. The DOUBLEHET module is capable of handling all the TRISO buffer layers of the fuel particles and the whole pebble at once [10]. Using the DOUBLEHET-module the ENDF-V5, V6 or V7 238-group libraries can be used.

In the first and most elaborate parameter study, the infinite multiplication factor has been calculated for different U-233 weight fractions, between 2% and 20%, and for different heavy metal loadings, ranging from 0.5 g to 30 g HM per pebble. The heavy metal loading of a fuel pebble is given by

$$m_{hm} = \frac{4}{3}\pi\rho_{hm}n_{triso}r_{fk}^{3}, \qquad \text{(eq. 1)}$$

where ρ_{hm} is the density of the heavy metal, n_{triso} the number of TRISO particles per pebble and r_{fk} the radius of the fuel kernel.

During the calculations, the heavy metal loading is increased by means of *either* an increase of the fuel kernel radius *or* an increase of the number of TRISO particles. So the change of k_{inf} can be compared for a large kernel size with respect to the standard size at the same heavy metal loading per pebble.

The influence on k_{inf} of adding moderator pebbles between the fuel pebbles is investigated in a second parameter study. Moderator pebbles can be added to change the moderation ratio of the fuel without making changes to the fuel pebble design itself. Fuel pebbles with a high heavy metal loading are used for this parameter study, since they are strongly undermoderated without moderator pebbles. In the next two subsections the results of the two different parameter studies are discussed and general trends of the parameter variations are analysed.

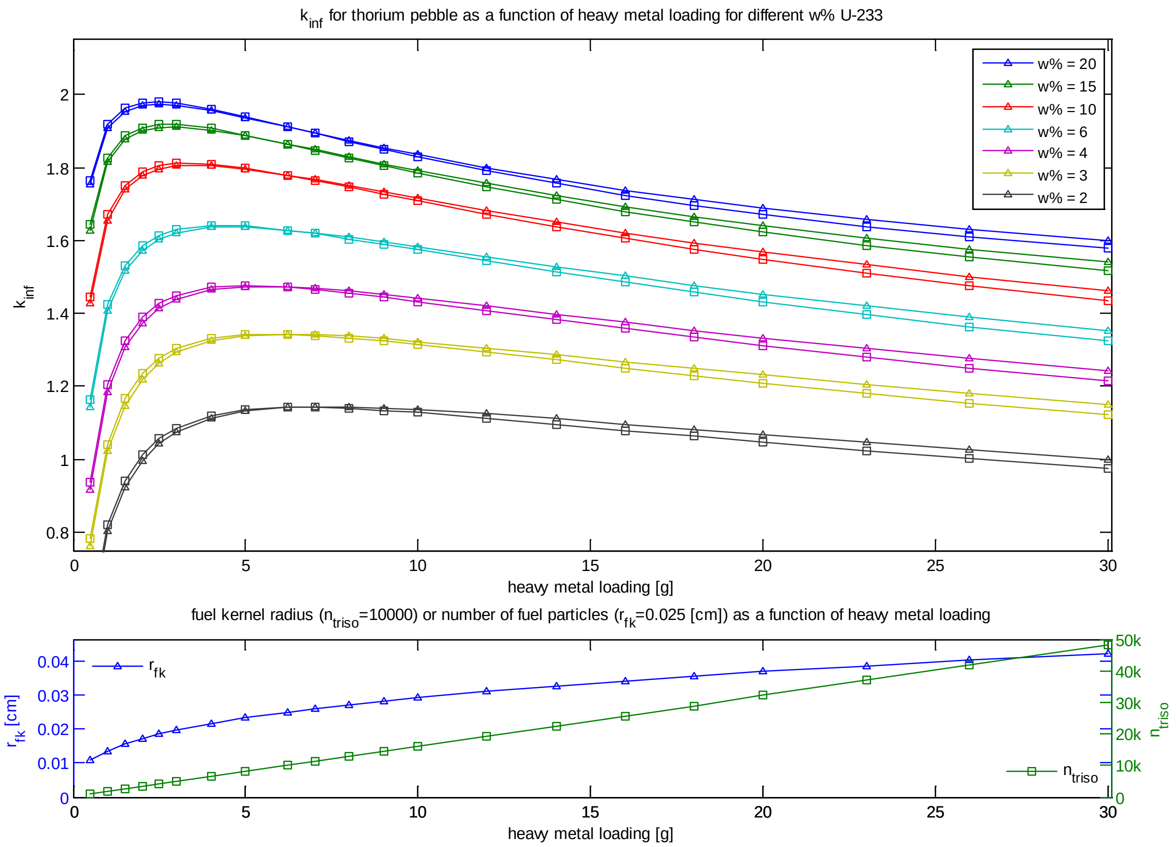

Fig. 1: k_{inf} of fresh fuel pebble as a function of heavy metal loading for different U-233 weight fractions (*top*) and for two different methods used for varying the heavy metal loading, either by increasing fuel kernel size – triangles – or number of TRISO particles – squares (*bottom*)

II.A. Varying Heavy Metal Loading

For the first parameter study the k_{inf} of the fresh Th/^{233}U-fueled pebble was calculated with the heavy metal loading being varied from 0.5 g to 30 g. In one case the heavy metal loading was varied by changing the fuel kernel radius in 21 steps between 0.1079 and 0.4224 mm, while 10000 TRISO particles were used per pebble. In the second case the heavy metal loading was also varied in 21 steps by changing the number of TRISO particles between 804 and 48249, while using a fuel kernel radius of 0.2500 mm. These calculations were performed for 14 different weight fractions of U-233 ranging from 2% till 20%. For this first parameter study the DOUBLEHET module of the CSASI sequence and the ENDF-V5 238 group library were used.

From the results, as shown in figure 1, it becomes clear that the magnitude of the heavy metal loading is of great importance for the pebble k_{inf}. The method by which the metal loading is varied, *either* by enlarging the fuel kernel *or* increasing the number of particles, is of smaller importance for the thorium fuelled pebble. This fuel lumping effect is clearly less significant for thorium than for U-238, since the resonances in the capture cross section of thorium are much smaller. The largest relative difference between the two methods is found at the highest metal loading (30 g) for a thorium fuelled pebble with 2 w-% U-233. The k_{inf} is 2.76% higher when an enlarged fuel kernel is used. As a reference it was found for a pebble (30 g HM) with 2% U-235 and 98% U-238 that the relative difference in k_{inf} is 5.90%.

The fuel pebble is overmoderated for low metal loadings. A slightly higher heavy metal loading leads to an increase of k_{inf}. The fuel pebble is undermoderated for high metal loadings and adding more fuel leads to a decrease of k_{inf}. The maximum of k_{inf} occurs at higher metal loadings for lower U-233 weight fractions. Since the ratio between carbon moderator and fissile material is already lower for a higher U-233 weight fraction, the pebble will already become undermoderated at a lower heavy metal loading.

With respect to the fuel design it can be noted that an increase of fuel self shielding leads to an increase of k_{inf}. It also results in a decrease of neutron capture in thorium and conversion into U-233. For the fuel design in a thorium high conversion pebble bed reactor choices should be made between these two opposite effects.

II.B. Adding Moderator Pebbles

The addition of moderator pebbles is the second parameter study performed for fresh fuel pebbles. The ratio of moderator to fuel pebbles, denoted by *f*, was varied between 0 and 10, for a fuel pebble with a 30 g heavy metal loading (n_{triso}=48249; r_{fk}=0.25 mm). Calculations were performed for a range of U-233 weight fractions between 2% and 20%. The 2REGION method [11] was used for the self shielding. The 2REGION method solves a slowing-down equation representing a system by an interior region containing the material mixture to be self-shielded and an outer moderator region. Using the 2REGION method a user specified Dancoff factor, depending on the amount of moderator pebbles present in the fuel, can be used to take into account the double-heterogeneity of the fuel. These Dancoff factors were calculated by means of the analytical equations derived by Bende et al. [12]. The cross section generation procedure used for a mixture of fuel pebbles and moderator pebbles has been described in the thesis work of Boer [13]. Cross sections are obtained from the ENDF-V7 238-group library. The k_{inf} is plotted as a function of *f* for 2, 2.5, 3 and 4 w% of U-233 in figure 2.

A fuel pebble (*f*=0) with a heavy metal loading of 30 grams is strongly undermoderated. For all weight fractions of U-233, the addition of moderator pebbles initially leads to an increase of k_{inf} until the moment the fuel pebble becomes overmoderated when *f* becomes larger. As the U-233 weight fraction increases the value of *f* at which the transition from undermoderated to overmoderated occurs also increases.

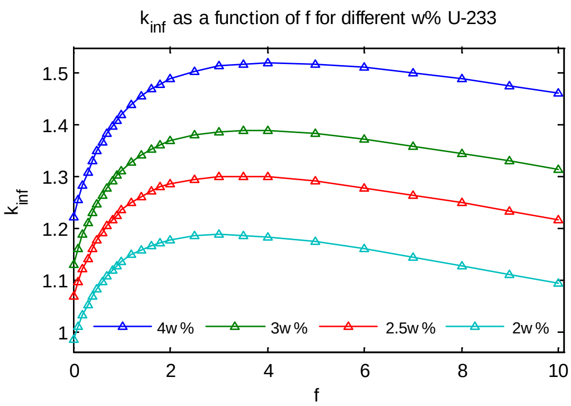

Fig. 2: k_{inf} as a function of moderator to fuel pebble ratio (*f*) for different U-233 w% (m_{hm}=30 g)

A significant increase of the pebble k_{inf} can be achieved by the addition of moderator pebbles. For a 3 w% U-233 fuel pebble (30 g HM) the addition of 3.5 moderator pebbles with each fuel pebble leads to an increase of k_{inf} from 1.1319 to 1.3902. The use of moderator pebbles offers the opportunity to increase k_{inf} of a pebble with a large heavy metal loading significantly without making changes to the fuel pebble itself.

III. PARAMETER STUDIES OF THORIUM PEBBLE BURNUP

The composition of the fuel inside the pebbles during depletion is an important aspect with respect to the choice of the fuel design of a thorium breeder pebble bed reactor. An accurate determination of the burnup of the fuel inside a reactor requires knowledge of the configuration of the whole reactor core, since this will determine the flux (and spectrum) inside the fuel during depletion. It is however not feasible to work with core configurations, as the fuel design is still to be determined. For this reason a simplified method has been developed to perform burnup calculations. It is important that the method is relatively fast in order to perform extensive parameter studies of the fuel design during burnup.

The average length a neutron travels before absorption is much longer inside a pebble bed reactor than the size of a single pebble. The neutron spectrum inside a pebble is therefore mainly determined by the composition of the surrounding pebbles. Usually the fuel pebbles in a pebble bed reactor are recycled multiple times into the core and of main interest is the reactor in equilibrium configuration. In that case, according to Massimo [14], all burnup stages of the fuel are represented in any volume element of the core and, because of the small size of the fuel elements, the neutron spectrum is determined by the average nuclide composition.

III.A. Calculational Method

For the burnup calculations several modules of the SCALE6 code package were used. As a first step the fuel depletion for a single pebble in an infinite lattice is calculated. Therefore an AMPX-library with zone weighted microscopic cross sections is generated by the CSASI-sequence for the nuclides in the fuel kernel of the pebble. For the unit cell calculation the ENDF-V5 238-group library has been used in combination with NITAWL for the self shielding calculation.

The AMPX-library is converted into an ORIGEN working library by COUPLE. Then ORIGEN-S is used to calculate the fuel depletion with a constant specific power during one burnup step. ORIGEN-S divides the depletion calculation for each burnup step again into several subintervals. After each burnup step, new nuclide concentrations are calculated for the fuel kernel from the ORIGEN-S output and a new AMPX-library is generated by the CSASI-sequence to provide the neutron spectrum inside the fuel kernel for the next depletion calculation step by ORIGEN-S. This process is repeated until the final burnup is reached. The k_{inf} of a fuel pebble at each burnup step is also extracted from the CSASI unit cell calculations.

As previously mentioned, the neutron spectrum inside a fuel pebble is mainly determined by the average composition of the surrounding pebbles. The spectral influence of these surrounding pebbles was not taken into account during the first part of the calculation. Using this first part of the calculation a cell-weighted macroscopic cross section set of a fuel pebble at middle of life (MOL) burnup is generated to represent MOL burnup pebble bed material. It is assumed that a pebble at a MOL burnup level is representative for the average nuclide composition of the surrounding pebbles.

The second part of the calculation is started with the generation of an AMPX-library with zone weighted microscopic cross sections by the CSASI-sequence for the fuel kernel. A separate CSASI calculation is run to generate macroscopic cross sections using an inner-cell weighting over the fuel zone. These two AMPX libraries and the MOL burnup pebble bed material cross sections are then merged together into one library using WAX.

With the cross sections of the different material regions a 1D transport calculation is performed with XSDRN for the pebble of interest surrounded by MOL burnup pebble material. The radius of the MOL pebble material is chosen to be large (200 cm) compared to the size of the pebble. In the center of the pebble of interest one separate fuel kernel is modelled in order to obtain zone-weighted cross sections for the fuel kernel material. In this way the neutron spectrum inside the fuel kernel is obtained with a good estimate of the influence of the MOL burnup surrounding pebbles.

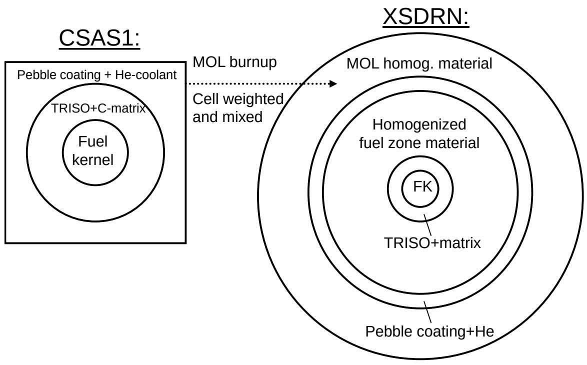

Fig. 3: Schematic view of burnup calculation method to capture influence of MOL burnup pebbles upon the fuel kernel spectrum

The fuel kernel cross sections generated by XSDRN are converted into an ORIGEN working library by COUPLE. Then ORIGEN-S is used to perform the depletion calculation over one burnup step. From the ORIGEN-S output new nuclide concentrations are determined and the above procedure is repeated to generate the new fuel kernel cross sections and neutron spectrum for the next burnup step. A schematic view of the geometry used for the cross section generation in the first and second part of the calculation is given in figure 3.

III.B. Influence of Pebble Environment in Fuel Depletion Scheme

Before discussing the complete set of results obtained by the burnup parameter studies of a fuel pebble, it is interesting to check the influence of using a single pebble spectrum or the inclusion of the MOL burnup material around the fuel pebble upon the results of the parameter studies.

The relative difference in k_{inf} or the nuclide concentrations has been defined by eq. 2 and eq. 3 in order to obtain a single quantative parameter to describe the relative difference between the use of a single or a MOL environment spectrum for a whole parameter set

$$\delta k_{\text{inf}} = \frac{\sum_{n_j} \left| k_{\text{inf,MOL}}\left(t_j\right) - k_{\text{inf,single}}\left(t_j\right) \right|}{\sum_{n_j} \left| k_{\text{inf,MOL}}\left(t_j\right) \right|}, \quad \text{(eq. 2)}$$

$$\delta N_i = \frac{\sum_{n_j} \left| N_{i,\text{MOL}}\left(t_j\right) - N_{i,\text{single}}\left(t_j\right) \right|}{\sum_{n_j} \left| N_{i,\text{MOL}}\left(t_j\right) \right|}. \quad \text{(eq. 3)}$$

Here n_j stands for the total number of burnup steps and j represents the j-th burnup step. 2D plots of the relative differences in k_{inf} and the U-233, Th-232 and Pa-233 nuclide concentrations, as defined by eq. 2 and 3 are shown in figure 4.

The influence of the use of the MOL environment for determination of the spectrum of the burnup calculations upon k_{inf} is for the largest part of the computational domain quite small for the ^{233}U/Th fueled pebbles, especially for the higher U-233 weight fractions. However, for pebbles with a metal loading between 5 and 15 grams and U-233 weight fraction between 5% and 10% the relative difference is greater than 1%. For pebbles with a large metal loading and low initial U-233 weight fraction the relative difference in k_{inf} can even become greater than 3%.

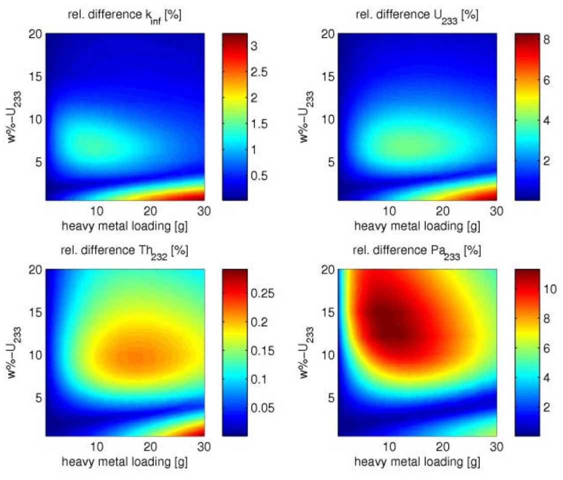

Fig. 4: Relative difference - in % - in k_{inf}, U-233, Th-232 and Pa-233 concentrations between the use of a MOL environment and a single pebble spectrum as a function of heavy metal loading and initial U-233 weight fraction

The relative differences in the Th-232 concentration are small. This is mainly because the absolute differences are small compared to the large amount of thorium available in the fuel. The relative differences in the Pa-233 and U-233 concentrations can be significant. The largest relative difference in the Pa-233 concentration is 11.3%. The largest relative difference, with a value of 8.28%, in the U-233 concentration is also found at a large metal loading and low initial U-233 weight fraction.

As a conclusion it can be stated that including the MOL spectrum into the calculations leads to small changes in k_{inf} and U-233 concentration for high initial weight fractions of U-233. For lower initial U-233 weight fractions the relative difference between a MOL spectrum and a single pebble spectrum becomes larger. This is especially the case when fuel pebbles with a large heavy metal loading and very low initial U-233 weight fraction are used. It will be shown in the next subsection that this type of fuel pebble is actually the most interesting for use in a thorium high conversion pebble bed reactor.

III.C. K_{inf} and Nuclide Concentrations as a Function of Heavy Metal Loading

A similar parameter study as for the fresh fuel pebble with varying heavy metal loading has been performed for U-233/Th pebbles during depletion. This time also initial U-233 weight fractions of 0.5%, 1.0% and 1.5% were used in the calculation. During the burnup calculation a specific power of 80 MW/t_{hm} is used. The burnup calculation is performed over 16 burnup steps, consisting of 10 intervals in the ORIGEN-S calculation. Each interval corresponds to a period of 10 days. The maximum burnup is 128 GWd/t_{hm} and the MOL burnup 64 GWd/t_{hm}.

The burnup calculations were performed for 21 different metal loadings, achieved by *either* varying the fuel kernel radius *or* the number of TRISO particles, and 17 different U-233 weight fractions. The possible increase in U-233 concentration, the Pa-233 concentration and k_{inf} are relevant indicators of the usefulness of the fuel inside the thorium (near) breeder pebble bed reactor. From this parameter studies it was found that a pebble with a high metal loading (and obviously a low initial w% U-233) can achieve the largest increase of the U-233 concentration.

The infinite multiplication factor, the U-233 and Pa-233 concentration are shown in figure 5 for the burnup calculation with MOL burnup environment of a pebble with an initial U-233 weight fraction of 0.5% and three different metal loadings. As a result of the constant specific power used by ORIGEN-S and the low initial fissile content of the fuel pebble a high neutron flux is used in the first stages of the burnup calculation by ORIGEN-S. The high neutron flux and large amount of capture in the thorium leads to a peak in the Pa-233 concentration at low burnup. Such a peak is not likely to occur in a real HTR core as the fuel depletion is driven by the flux inside the core.

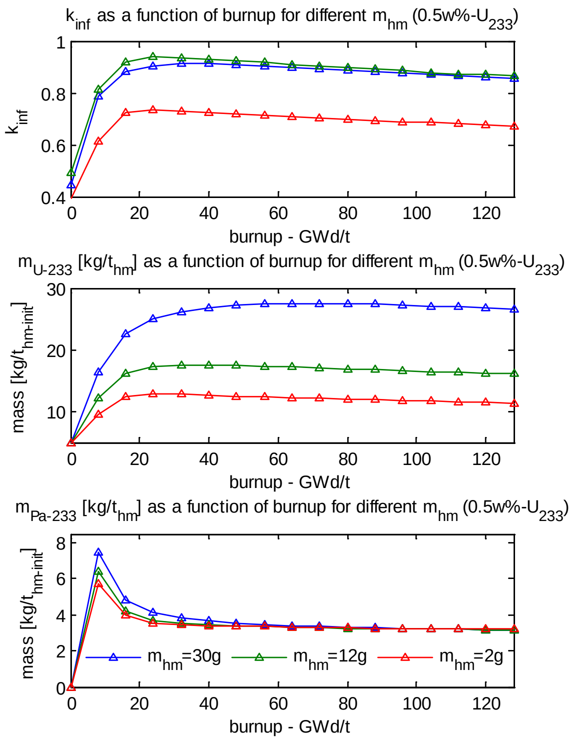

Fig. 5: k_{inf}, U-233 and Pa-233 concentrations as a function of burnup for different metal loadings per pebble using an initial U-233 weight fraction of 0.5% and 80 MW/t_{hm} specific power

For all the pebbles with 0.5% initial U-233 weight fraction the k_{inf} remains below 1. This can be improved by including decay intervals for Pa-233 during the burnup. In this way less neutrons are lost in the strongly absorbing Pa-233 and a larger fraction of Pa-233 can be converted into the fissile U-233. For the pebbles with high metal loading k_{inf} can be increased by adding moderator pebbles. This enables the creation of an undermoderated breeding zone and a more optimally moderated driver zone. The possible effect of adding moderator pebbles upon pebble k_{inf} has been demonstrated for the 30g HM fresh fuel pebble.

It was also found that for most of the pebbles the U-233 concentration at final burnup is roughly the same for all the different U-233 initial weight fractions, except for the really high initial U-233 weight fractions. In that case the fuel has not depleted far enough as the maximum burnup is reached.

For the fresh fuel pebble it was found that the method by which the metal loading is varied (*either* by enlarging the fuel kernel *or* increasing the number of particles) is of much smaller importance than the magnitude of the heavy metal loading itself. The parameter studies of the burnup of the fuel pebble indicate that the differences in k_{inf} between *either* increasing kernel size *or* number of coated particles tend to become smaller with increasing burnup.

At the maximum burnup the difference in k_{inf} between the two methods for a 30 g HM pebble with 0.5 initial w% U-233 is only 0.28%. However for the same pebble the U-233 concentration at maximum burnup is 24.736 kg/t_{hm} (r_{fk}=0.4224 mm, n_{triso}=10000) compared to 26.598 kg/t_{hm} (r_{fk}=0.25 mm, n_{triso}=48249). This corresponds to a difference of 7.53%. The self shielding effect is smaller inside a fuel pebble with a larger amount of smaller fuel kernels. Consequently more neutron capture inside thorium occurs and therefore the U-233 concentration at final burnup is higher. The negative effect of the increased neutron capture is that less neutrons are available for new fission reactions. Apparently the increased amount of fissile material and the lower availability of neutrons for fission almost balance each other out.

III.D. Burnup for Varying Specific Power

During the parameter study performed in the previous subsections a specific power of 80 MW/t_{hm} was used. The use of a higher or lower specific power can have a significant impact upon k_{inf} and the U-233 and Pa-233 concentrations. It influences the rate of Pa-233 production by means of neutron capture in thorium and changes the time scale available for Pa-233 to decay into U-233. The specific power during fuel burnup could also be a relevant parameter to optimize with respect to the conversion from thorium into U-233.

Using the 30 g HM 0.5 initial w% U-233 pebble, the burnup calculation has been performed for eight different specific powers between 5 MW/t_{hm} and 800 MW/t_{hm}. In figure 6, the k_{inf} and the U-233 and Pa-233 concentrations are shown for specific powers of 20, 80 and 400 MW/t_{hm} as a function of burnup. Again the peak in the Pa-233 concentration is a result of the large flux required during the early burnup stages to obtain a constant power for the fuel pebble with a low initial fissile loading.

The use of a high specific power for the 30 g HM pebble with 0.5 w% U-233 leads to a strong increase of the Pa-233 concentration, because more neutrons are captured by thorium. The time required to reach a certain burnup level is much shorter if a higher specific power is used. Consequently Pa-233 has much less time to decay to U-233, and the increase of k_{inf} and U-233 concentration is much slower as a function of burnup if a high specific power is used.

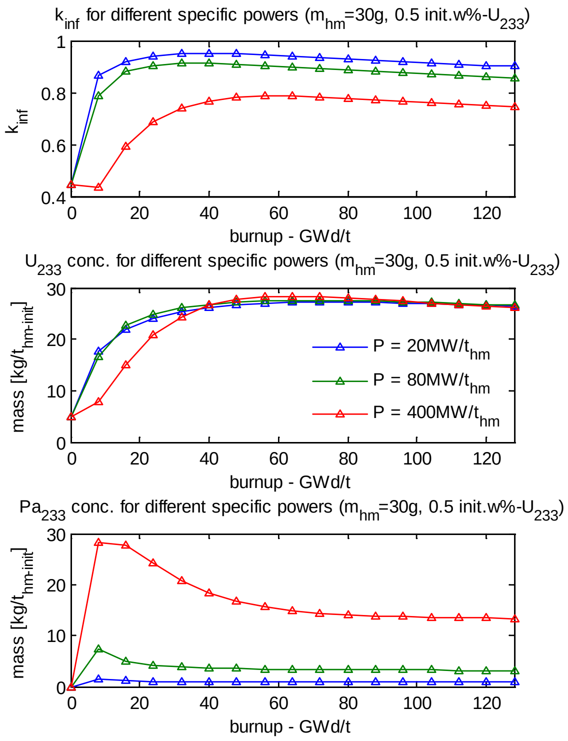

Fig. 6: k_{inf}, U-233 and Pa-233 concentrations as a function of burnup using varying specific powers for a 30 g heavy metal loaded pebble using an initial U-233 weight fraction of 0.5%

For specific powers lower than 80 MW/t_{hm} the maximum concentration of U-233 during burnup is not significantly different from the 80 MW/t_{hm} case. But the Pa-233 concentration is lower and less neutrons are captured in the Pa-233. As a consequence the k_{inf} of the pebble irradiated with a lower specific power is quite a bit higher. From the results it can be concluded that for a specific power between 5 MW/t_{hm} and 160 MW/t_{hm} the differences in the U-233 concentration as a function of burnup are quite small, but k_{inf} becomes higher as a lower specific power is used.

IV. REACTIVITY COEFFICIENTS

Uniform, moderator and fuel temperature reactivity coefficients have been determined for Th/^{233}U fuelled pebbles in an infinite lattice. Therefore k_{inf} values have been compared after a temperature change, from 1100 to 1300 K, of the whole pebble, the graphite and the fuel kernel respectively.

Similar to the calculations in section II.B, the addition of moderator pebbles is modelled by expanding the graphite shell around a pebble with the volume of the moderator pebbles. However, the calculations were performed with the DOUBLEHET module instead of the 2REGION method in SCALE6. With the 2REGION method convergence difficulties in the XSDRN calculation were sometimes encountered for certain temperatures and higher heavy metal loadings. This was not a problem using the DOUBLEHET module and similar results were found.

For the calculations a 2.5% weight fraction of U-233 is used, as this value compares well with the build-up of the U-233 weight fraction found in the depletion calculations.

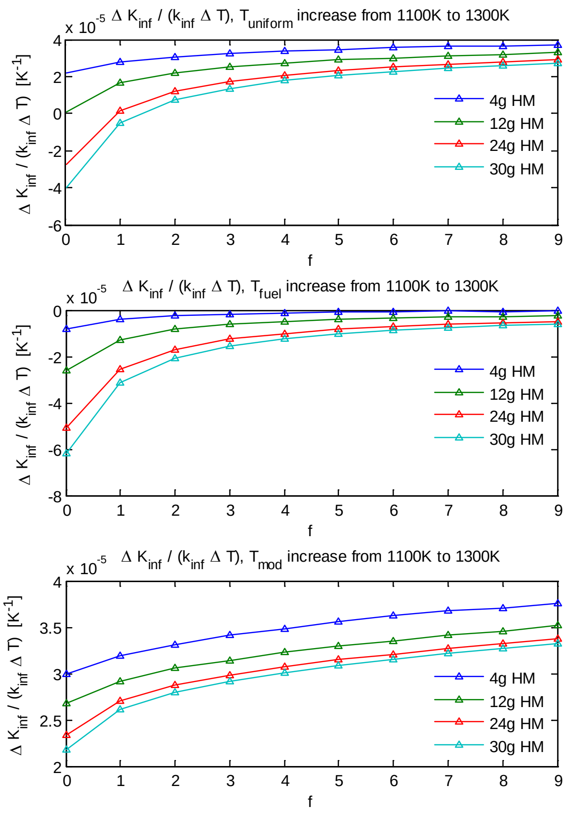

Fig. 7: Uniform, fuel and moderator temperature reactivity feedback of Th/^{233}U pebbles as a function of moderator to fuel pebble ratio (*f*) for different heavy metal loadings and a 2.5% U-233 weight fraction.

The uniform, fuel and moderator temperature reactivity feedback ($\frac{1}{k_{\text{inf}}}\frac{\Delta k_{\text{inf}}}{\Delta T}$) of Th/^{233}U pebbles are plotted as a function of the moderator to fuel pebble ratio for different heavy metal loadings in figure 7.

In all cases the fuel temperature or Doppler feedback is negative. The moderator temperature coefficient is however positive in all cases. For solid-moderated cores an increase of the moderator temperature leads to a hardening of the thermal neutron spectrum [3]. For ^{233}U/Th fuelled cores the peak in the thermal neutron spectrum is shifted into an energy region where the ratio of fission in U-233 over absorption in Th-232 increases causing a positive moderator temperature feedback. This phenomenon has also been described by Nuttin et al. [15] for a thorium molten salt reactor with graphite moderator and reflectors.

Without moderator pebbles, the uniform temperature coefficient is only negative for heavy metal loadings larger than 12 g. If one moderator pebble is added for each 24 g HM pebble a similar uniform coefficient is found as for the 12 g HM pebble as the moderator-to-fuel ratio in both cases is the same. For the 30 g HM pebble, which yielded the optimal thorium to U-233 conversion in the depletion calculations, only slightly more than one moderator pebble may be added per fuel pebble to maintain a negative uniform temperature coefficient.

It should however be noted that these calculations were only performed for a single Th/^{233}U pebble with white boundary conditions. It remains to be seen how neutron leakage and reflectors influence the temperature coefficients in a finite reactor geometry.

V. CONCLUSIONS

In this work fuel design studies have been performed for fresh thorium pebbles and during depletion. For the depletion calculations a calculational scheme was used where middle-of-life burnup pebble cross sections were used as a surrounding material. This way a more realistic neutron spectrum was provided for the depletion calculations by ORIGEN. The MOL spectral environment has a significant influence on k_{inf} and the U-233 concentration, in case of very low initial U-233 weight fractions and large heavy metal loadings.

The results of the fuel design studies presented in this work can be used as a basis for future core design and fuel management studies of a thorium fuelled (near) breeder pebble bed reactor. Such a core can consist of one or multiple breeder zones and one or multiple driver zones.

The breeder zones are loaded only with thorium pebbles with a large heavy metal loading (30 g), and its fuel particles have the standard fuel kernel radius of 0.025 cm. For these pebbles the highest possible thorium to U-233 conversion could be achieved during the depletion calculations.

Following the irradiation in the breeder zone and a certain decay period for the Pa-233, the fuel pebbles can be recycled, one or multiple times, into a driver zone. The driver zone consists of a mixture of fuel and moderator pebbles. The addition of moderator pebbles reduces resonance absorption and raises k_{inf} above one, without reprocessing of the fuel.

Only slightly more than one moderator pebble per fuel pebble may be added to maintain a negative uniform temperature coefficient. However, the influence of reflectors and neutron leakage, in a finite reactor geometry, remains to be investigated.

For a better neutron economy, reactor powers should not be too high in order to reduce parasitic capture in Pa-233.

ACKNOWLEDGEMENTS

The authors like to thank D. Rodríguez for his assistance with the reactivity coefficient calculations in section IV.

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