

MODELLING OF HTRs: FROM A HOMOGENOUS TO AN EXACT HETEROGENEOUS CORE WITH MONTE CARLO

Danas RIDIKAS and Rita PLUKIENE for the Mini-Inca project
DSM/DAPNIA/SPhN, CEA Saclay
F-91191 Gif-sur-Yvette, France
ridikas@cea.fr

ABSTRACT

The gas turbine modular helium-cooled reactor (GT-MHR) is known probably as the best option for the maximum plutonium destruction in once-through cycle, even though the industrial fabrication of coated particle fuel still has to be proved. We perform detailed Monte Carlo simulations along these lines by comparing different geometry sets, namely homogenous versus single-heterogeneous and double-heterogeneous, in terms of k_{eff} eigenvalues, the length of the fuel cycle, neutron characteristics and the evolution of fuel composition in particular. In all cases the same MonteBurns code system is used. We show that the performance of GT-MHR may be considerably influenced by the way its geometry is modelled within the Monte Carlo approach.

1. INTRODUCTION

Gas-cooled reactor technologies (e.g. GT-MHR [1]) seem to offer significant advantages in accomplishing the transmutation of plutonium isotopes and nearly total destruction of ^{239}Pu in particular. GT-MHR uses a variable in time neutron spectrum, operates at high temperature and employs ceramic-coated fuel. It utilises natural erbium as a non-fertile burn-able poison with the capture cross section having a resonance at a neutron energy such that ensures a strong negative temperature coefficient of reactivity. The lack of interaction of neutrons with coolant (helium gas) makes sure that temperature feedback is the only significant contributor to the power coefficient. As a matter of fact, no additional plutonium is produced since no ^{238}U is used. A gas-cooled high temperature reactor or a separate irradiation zone in the centre of GT-MHR assembly, coupled to an accelerator [2], could also provide a fast neutron environment due to the same reason -- the helium coolant is essentially transparent to neutrons and does not change neutron energies. Since other actinides with an exception of plutonium are more inclined to fission in a fast neutron energy spectrum, one could consider an additional fast stage, following a thermal stage, in order to eliminate the remaining actinides [2].

In this paper we will describe in detail the use of a critical GT-MHR for transmutation of Pu isotopes from military applications. We note separately that a similar study with civil plutonium as a fuel has also been carried out but to be reported elsewhere due to limited size of this manuscript. The main goal of our study is to compare the performance parameters of the reactor core in the once-through cycle as a function of different geometry representation, i.e. homogeneous, single-heterogeneous and double-heterogeneous within Monte Carlo approach. MonteBurns [3], namely a coupled MCNP [4] and ORIGEN [5] code system, is employed at different stages of our simulations. The performance of it has been successfully benchmarked in Ref. [6] by simulating the fuel cycle of the high flux reactor at ILL Grenoble. We note that similar problematic (homogenous versus heterogeneous) was already

addressed in part in Ref. [7] but with different modelling schemes, e.g. a deterministic approach and/or based on the neutron diffusion theory.

2 MODELLING PROCEDURE

A simplified 3D model of GT-MHR reactor, which is shown in Fig. 1A, has been created using MCNP geometry set-up. Further details on this homogenous geometry modelling including some burn-up calculations can be found in [8]. We also refer to Refs. [9,10], where a comparative analysis of different data libraries and corresponding influence on the performance of a homogeneous GT-MHR has also been reported.

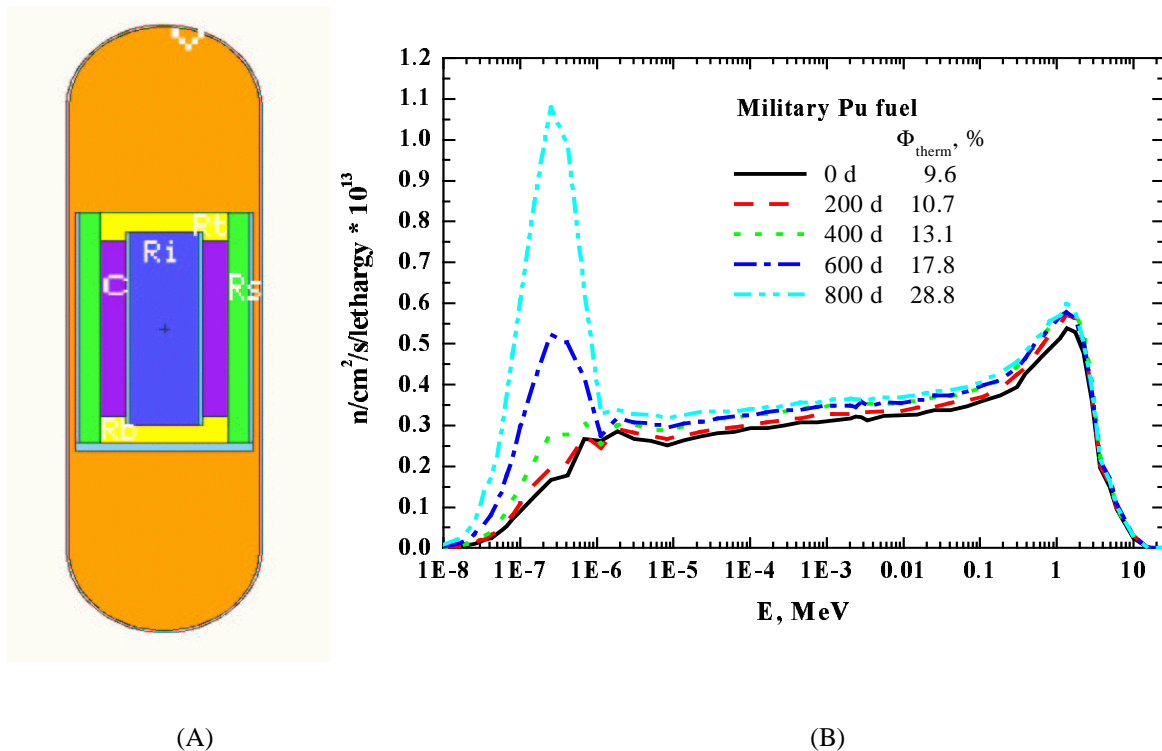


Figure 1: A) Length-wise section view of GT-MHR reactor model. The following notation is employed: C – active core (~8 m high), Rt - top reflector, Ri – inner reflector, Rb - bottom reflector, Rs - side reflector, and V - reactor vessel. B) Typical change of the average energy spectra of neutrons in the active homogenous core of GT-MHR for different fuel burn-up expressed in full power days.

In this work we also used MCNP to obtain k-eigenvalues and neutron fluxes. As soon as $k_{\text{eff}} < 1$ the length of the fuel cycle is determined in the case of a critical system. A typical neutron spectrum evolution for Pu fuel poisoned with natural Er is shown in Fig. 1B. The observed increase of the thermal flux from 10% to 30% is due to the loss of ^{239}Pu and ^{240}Pu in addition to the loss of the burnable poison during the operation. Indeed, the change of the energy spectra of neutrons will change the average cross sections to be used in the burn-up calculations, in some cases by a factor of two or more [8]. Therefore fuel evolution calculations have to be performed with corresponding variable neutron fluxes as it is done with Monteburns [3]. We note also that at the constant reactor power typical averaged GT-MHR neutron fluxes in the active core may increase by 50-100 %, i.e. from $\sim 1 \times 10^{14}$ n/(cm² s) to $\sim 2 \times 10^{14}$ n/(cm² s) at the beginning and at the end of the fuel cycle respectively [8].

3. HOMOGENEOUS AND HETEROGENEOUS GT-MHR

3.1 MAJOR GEOMETRY AND MATERIAL CHARACTERISTICS

As it was mentioned above, our major interest in this study was to look at the GT-MHR performance parameters by investigating three different geometry configurations: homogeneous (HTR0^{*}), single-heterogeneous (HTR1^{*}) and double-heterogeneous (HTR2^{*}).

The cross sectional view of the first type geometry, namely a homogeneous GT-MHR, is presented in Fig. 2A. Both geometry and materials have been fully homogenised as presented in the same figure. A single-heterogeneous GT-MHR includes hexagonal lattice structure (see Fig. 2B). Active core consists of 102 hexagonal prism columns located around the inner reflector (37 columns) and reflector with B₄C (24 columns). Side and permanent reflectors are constructed from graphite columns in the same manner around the active core. All corresponding material compositions were homogeneously distributed with specific material density for corresponding zones. Double-heterogeneous geometry feature is an explicit active core structure (see Fig. 3A.). In this case each hexagonal core column consists of 202 cylinders with fuel material, 14 cylinders with natural erbium and 108 cylinders with helium as it is shown in Fig. 3B. We did not model here the influence of ceramic-coated fuel and erbium particles. All of them were homogeneously placed in the silicon - graphite matrix in the form of homogenised compacts. We note separately that in all three cases (HTR0, HTR1 and HTR2) total mass of all materials taken separately was preserved (also see Table I).

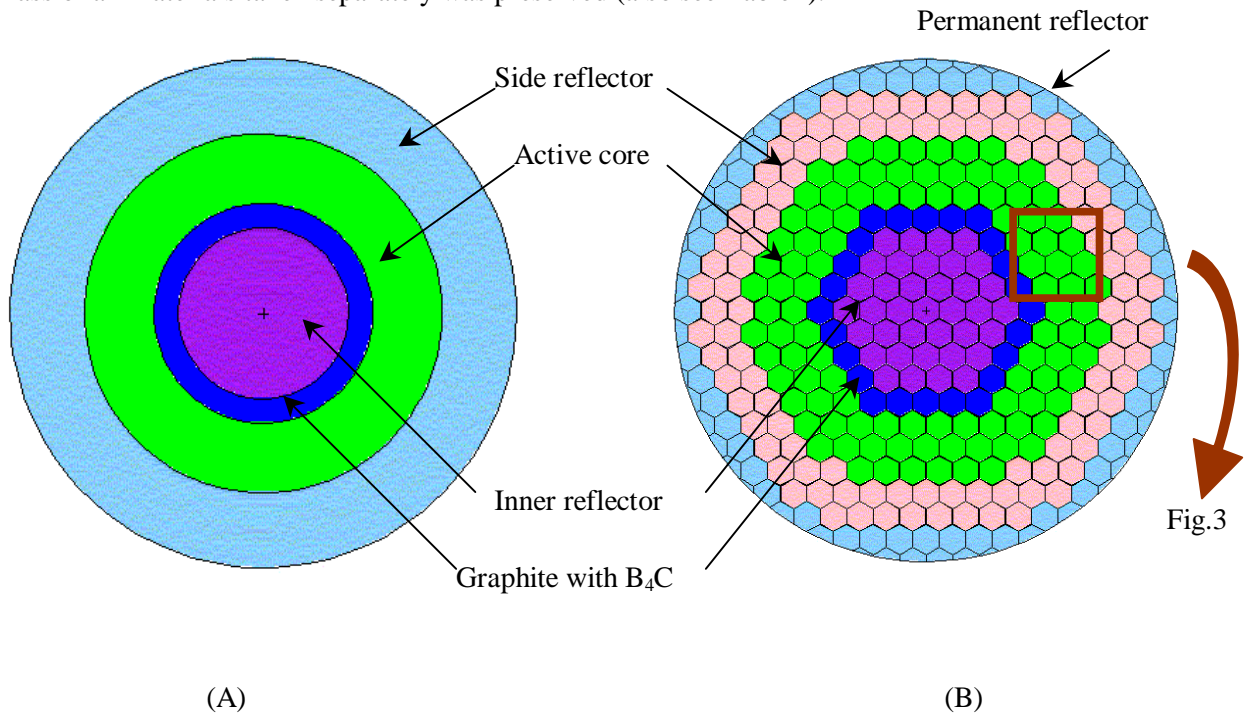


Figure 2. A cross section of the GT-MHR core: A) fully homogeneous core without hexagonal structure (HTR0); B) single-heterogeneous core with hexagonal prism lattice structure (HTR1).

* The same notation will be kept all over this paper.

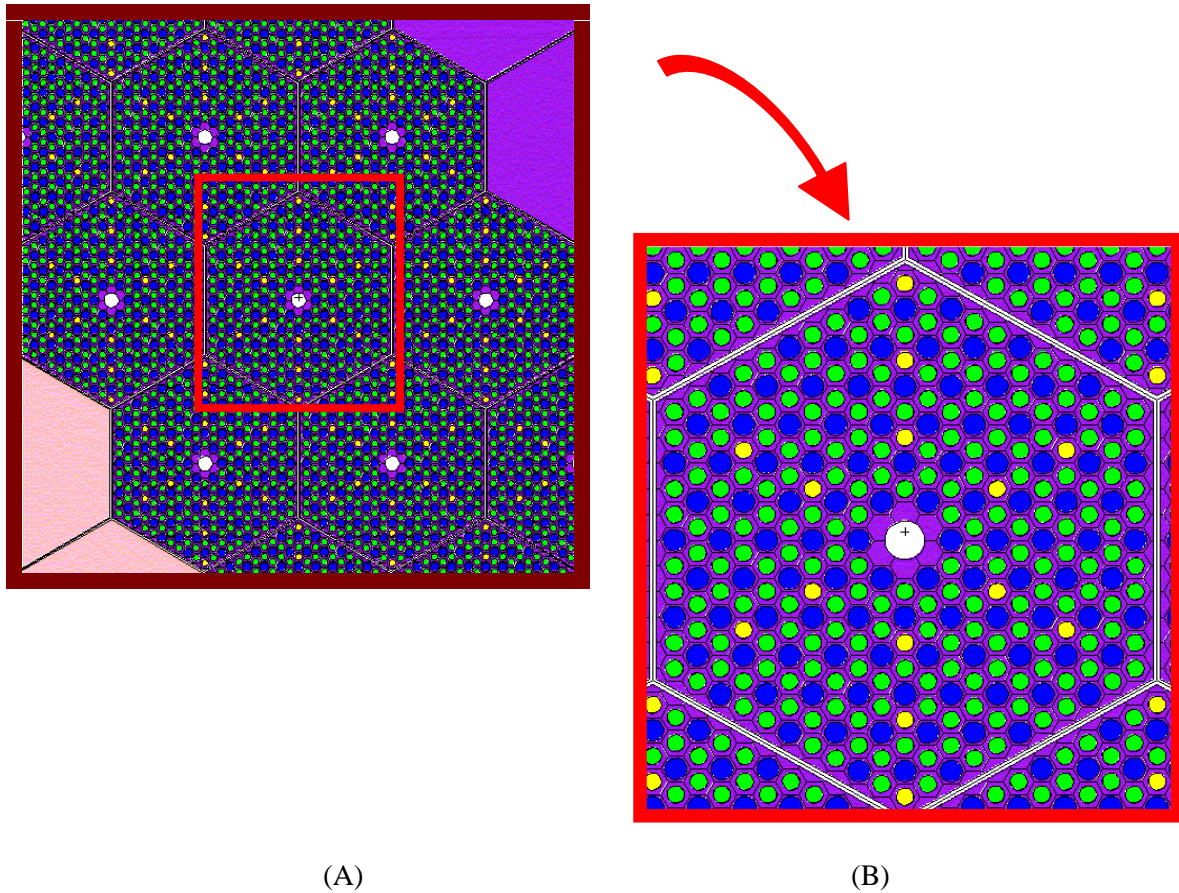


Figure 3. Fragments of double-heterogeneous GT-MHR (HTR2): A) an active core structure: three rings of hexagonal fuel assembly columns; B) magnified view of a separate fuel assembly. Fuel compacts are presented in green, burn-able poison compacts – in yellow. Blue holes stand for He channels, while the remaining violet colour represents the graphite matrix.

The main parameters used for modelling of three reactor designs are summarised in Table I. Note that in all cases the same conditions were kept.

Table I. Basic GT-MHR reactor parameters.

Simulation models	HTR0	HTR1	HTR2
Power, MW _{th}	600	600	600
Active core size:			
- height, cm	800.0	800.0	800.0
- area, m ²	11.5	11.5	11.5
Active core volume, m ³ :	91.9	91.6	91.6
Graphite mass in reactor, t:	616.3	616.3	616.9
Averaged temperature, °C:			
- active core	800		
- inner reflector	730		
- side, top and bottom reflectors	500		

We utilised the Monteburns code in all three cases. ENDF data library (as the most often employed with MCNP) was used for the fuel and structure materials, JENDL data files (having a biggest number of fission products) were employed for fission products. The initial fuel and burn-able poison composition is presented in Table II. In the case of military plutonium the following isotopic vector was taken: 94.0 % of ^{239}Pu , 5.4 % of ^{240}Pu and 0.6 % of ^{241}Pu .

Table II. Major GT-MHR material compositions.

Material	Military Pu
Isotopic fuel composition, kg :	
^{238}Pu	-
^{239}Pu	659.0
^{240}Pu	37.8
^{241}Pu	4.2
^{242}Pu	-
Total plutonium, kg :	701.0
Isotopic burn-able poison composition, kg :	
^{166}Er	138.0
^{167}Er	94.2
^{170}Er	61.4
Total erbium, kg :	293.6

3.2 K_{eff} and BURNUP RESULTS

We perform the calculations simulating the once-through fuel cycle scenario at the constant 600MW_{th} power. The length of the fuel cycle is determined according to the following criterion: $k_{\text{eff}} \geq 1$. In Fig. 4 we compare the behaviour of k_{eff} as a function of time (consequently, as a function of burn-up).

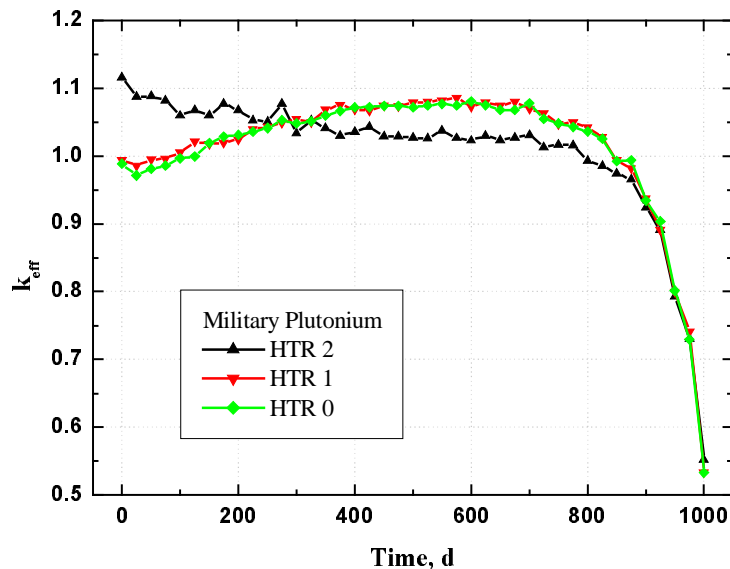


Figure 4. A behaviour of k_{eff} for different GT-MHR modelling cases with military plutonium fuel.

In the case of HTR0 and HTR1 k_{eff} drops below 1 approximately after 850 days, while the fuel cycle of HTR2 is somewhat shorter (~800 days). The dependence of k_{eff} also significantly differs only in the case of a double heterogeneous geometry HTR2. At the beginning $k_{eff} = 1.116 \pm 0.005$, 0.994 ± 0.005 , and 0.988 ± 0.005 for HTR2, HTR1 and HTR0 correspondingly. In addition, for HTR2 the curve of k_{eff} is constantly decreasing. Contrary, HTR1 and HTR0 corresponding curves first increase and decrease later on as a function of burn-up (see Fig. 4 for details). This major difference is explained by different burning of burn-able poison – erbium as shown in Fig. 5. It is clearly seen that erbium is consumed much faster in the case of a homogenous geometry-material specification, giving

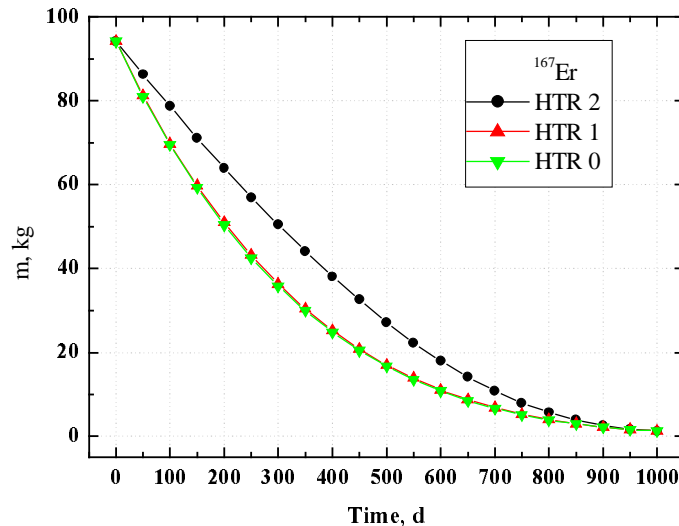


Figure 5. Burn-up of ^{167}Er as a function of irradiation in the case of HTR0, HTR1 and HTR2.

the answer why in these cases an average neutron capture cross section σ_c is different. Indeed, as it is shown explicitly in Table III both for HTR1 and HTR2 σ_c is much higher than for HTR0. It is important to note that this difference decreases with time due to the burn-up of ^{167}Er itself.

Table III. Capture and fission cross sections for different GTM-HR configurations

Element	^{167}Er σ_c , barns			^{239}Pu σ_f , barns		
	HTR2	HTR1	HTR0	HTR2	HTR1	HTR0
Time, d						
0	145	252	248	72.6	77.7	74.2
200	172	284	286	85.6	95.6	96
400	227	338	335	111	131	127
600	320	416	410	159	188	183
800	493	563	557	267	305	299

Contrary to the ^{167}Er capture cross section, the ^{239}Pu fission cross section is rather similar for all geometries considered. For this reason a corresponding evolution of ^{239}Pu (actually of all Pu isotopes) is also very similar as shown explicitly in Fig. 6. To explain this situation one needs only to remember the way all three geometries were modelled. In the case of HTR2 Er and Pu are burned in different neutron fluxes since these materials are in different cylindrical cells – compacts. Contrary, in the case

of HTR0 and HTR1 both Er and Pu are irradiated in the same neutron environment defined by the same geometrical cells.

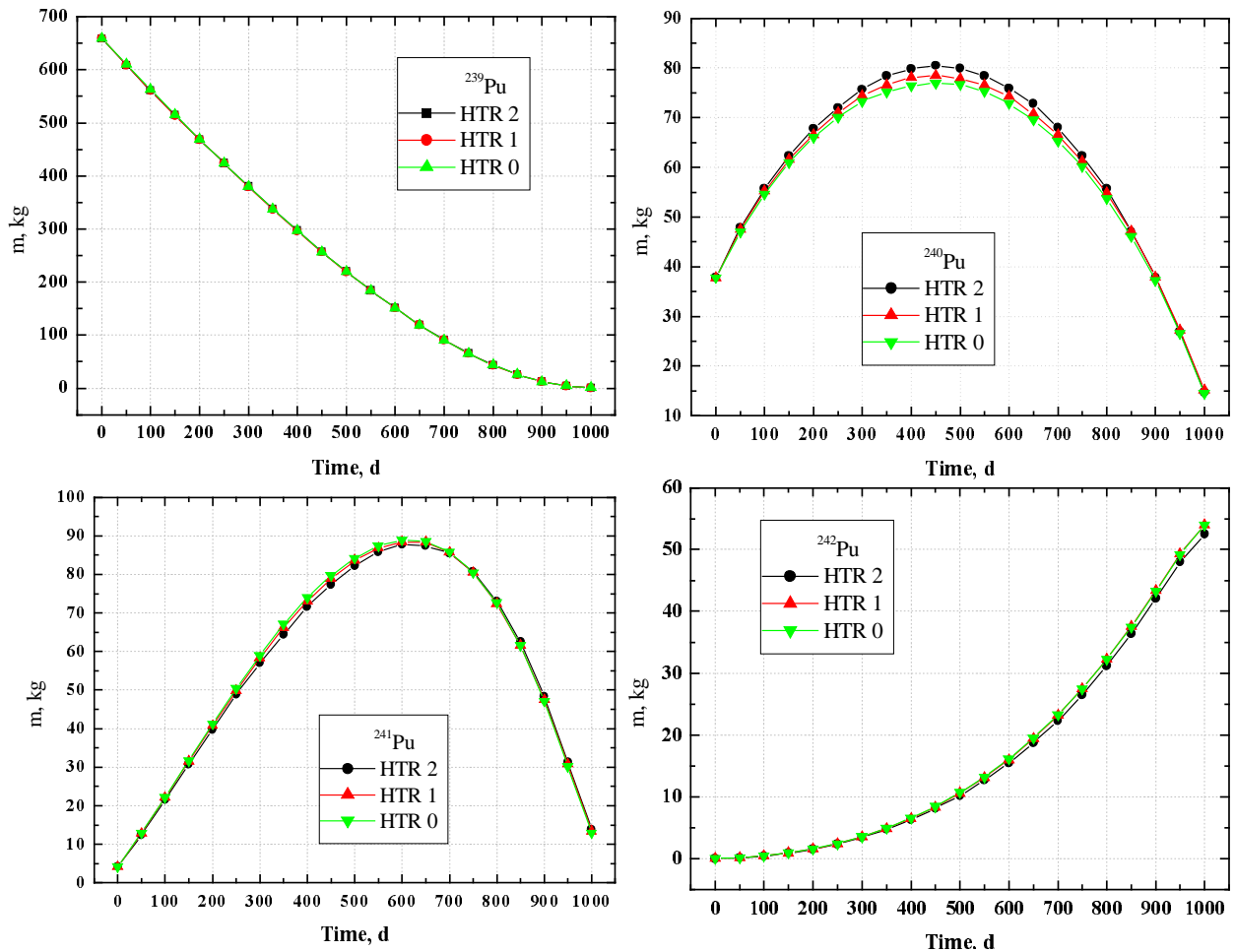


Figure 6. Evolution of mass for ^{239}Pu , ^{240}Pu , ^{241}Pu and ^{242}Pu for different GT-MHR modelling cases.

To clarify the situation even further in Fig. 7 we presented averaged neutron fluxes for all geometries considered both in the beginning and at the end of irradiation. Neutron fluxes “seen” by Er and Pu are presented in separate graphs on the left (7A) and on the right (7B) respectively. It is clearly seen that at the beginning a thermal neutron (up to 1 eV) contribution is bigger in HTR1 and HTR0 cases (~10 %), and is less in the case of HTR2 (~7 %). This is true in particular in the resonance region where neutrons are suppressed by the presence of Er in high concentration. After 800 days of operation the thermal neutron contribution is nearly the same in all cases due to the disappearance of ^{167}Er . We remind that in the case of HTR2 Er is located in a few particularly positioned cylinders – compacts (see yellow circles in Fig. 3B) what determines different internal characteristics compared with other cases. On the other hand, neutron spectra in the cells containing fuel are quite similar as shown in Fig. 7B. Even in the case of double-heterogeneous geometry only a small difference is observed due to a high number of fuel compacts (see green circles in Fig. 3B) what “homogenises” the system indirectly. The same conclusions are drawn both from one-group cross section calculations (Table III) and consequently from the fuel burn-up results (see Fig. 6). For example, after 800 days of irradiation the remaining mass of ^{239}Pu is 43.8kg, 43.5kg and 43.6kg in the case of HTR2, HTR1 and HTR0

respectively. The masses of other actinides at the end of the fuel cycle are given explicitly in Table IV.

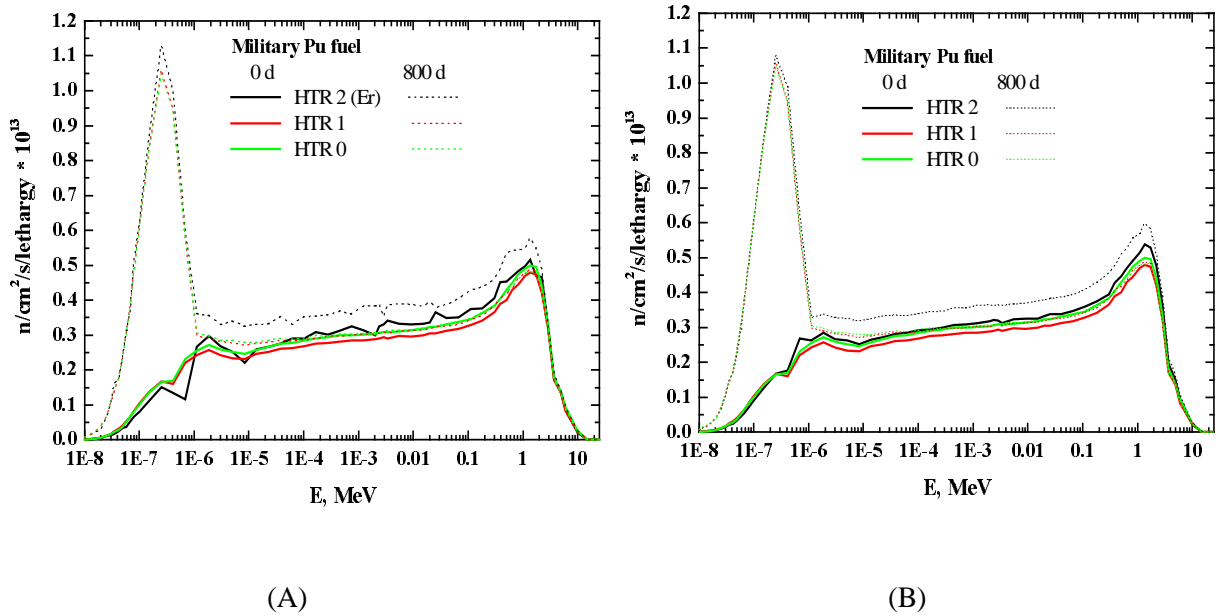


Figure 7. A) Neutron flux spectrum in burn-able poison cells for different GT-MHR modelling cases at the beginning and at the end of the fuel cycle. B) Same as in A but in the fuel material cells.

Table IV. The fuel and Er isotopic composition at the beginning and at the end of the fuel cycle.

Reactor geometry		HTR2	HTR1	HTR0
Time, days	0	800		
Fluence, n/cm ²		1.26×10 ²²	1.10×10 ²²	1.13×10 ²²
Actinides	Mass, kg			
²³⁸ Pu	0.0	1.3	1.3	1.3
²³⁹ Pu	659.0	43.8	43.5	43.6
²⁴⁰ Pu	37.8	55.7	54.9	53.7
²⁴¹ Pu	4.2	73.0	72.4	72.7
²⁴² Pu	0.0	31.2	32.3	32.3
²⁴¹ Am	0.0	2.5	2.6	2.6
²⁴² Am	0.0	<0.5	<0.5	<0.5
²⁴³ Am	0.0	4.6	4.3	4.5
²⁴² Cm	0.0	1.6	1.6	1.6
²⁴³ Cm	0.0	<0.5	<0.5	<0.5
²⁴⁴ Cm	0.0	1.9	1.5	1.6
²⁴⁵ Cm	0.0	<0.5	<0.5	<0.5
Total	701.0	216.0	215.0	214.0
Burnable poison	Mass, kg			
¹⁶⁷ Er	94.2	5.7	4.0	3.9

CONCLUSIONS

A critical GT-MHR dedicated to burn Pu isotopes in the once-through fuel cycle was studied comparing its performance parameters as a function of different geometry descriptions: homogeneous HTR0, single-heterogeneous HTR1 and double-heterogeneous HTR2. We have shown that it is very important to model the reactor geometry as precise as possible in order to characterise properly the performance of the system (e.g., k_{eff} , its behaviour with time and the length of the fuel cycle) although the fuel evolution results being very little dependent on the modelling procedure. The following conclusions are drawn:

1. A significant difference was found in k_{eff} values between HTR2 and HTR1 (equally HTR0) both at the beginning of the fuel cycle as well as in its evolution as a function of burn-up. HTR2's k_{eff} begins at higher value and it decreases constantly. Contrary, HTR1's and HTR0's k_{eff} begins at much lower value, increases to its maximum and later decreases.
2. A different behaviour of k_{eff} is explained by different modelling of burn-able poison (homogenous versus heterogeneous distribution). Consequently, the burn-up of erbium is rather different during the fuel cycle.
3. An exact modelling of the fuel compacts in the heterogeneous case in comparison with their homogeneous distribution does not have a big influence on neutron spectrum in the corresponding cells. This can be explained by a much bigger number of fuel compacts compared to the number of compacts containing burn-able poison.
4. Consequently, the evolution of military plutonium fuel at constant reactor power is very similar for all three geometry configurations.

Finally we add that a further step towards an exact geometry description with Monte Carlo would be to take into account precisely a coated particle structure inside the fuel and burn-able poison compacts. The work along these lines is in progress.

ACKNOWLEDGEMENTS

We would like to dedicate this work to Povilas GOBERIS (1976-2001).

REFERENCES

1. "Gas Turbine-Modular Helium Reactor (GT-MHR) Conceptual Design Description Report", No. **910720**, Revision 1, General Atomics, GA Project No.7658, July 1996, San Diego, USA.
2. C. Rodriguez et al., "The Once-through Helium Cycle for Economical Transmutation in Secure, Clean and Safe Manner", paper 72 in the *Proceedings of the 6th OECD/NEA Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation*, Madrid, Spain, 11-13 December 2000.
3. H. R. Trellue and D.I. Poston, "User's Manual, Version 2.0 for MonteBurns, Version 5B", LANL preprint **LA-UR-99-4999** (1999); H.R. Trellue, private communication, April 2000.
4. J.F. Briesmeister, "MCNP - A General Monte Carlo N-Particle Code", Technical Report LA-12625-M, LANL (1997).
5. RSIC Computer Code Collection, "ORIGEN 2.1 - Isotope Generation and Depletion Code Matrix Exponential Method", RSIC report CCC-371 (1991).
6. D. Ridikas et al., "On the Fuel Cycle and Neutron Fluxes of the High Flux Reactor at ILL

- Grenoble”, *Proceedings of the 5th Int. Specialists Meeting SATIF-5*, OECD/NEA, Paris, France, 17-21 July 2000.
7. F. Damian, “Capacity Analysis of HTRs in terms of utilisation of fissile materials”, CEA Saclay, report **CEA-R-5981** (PhD thesis in French) 2001.
 8. D. Ridikas et al., “Critical and Sub-Critical GR-MHRs for Waste Disposal and Proliferation-Resistant Plutonium Fuel Cycles”, paper 71 in the *Proceedings of the 6th OECD/NEA Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation*, Madrid, Spain, 11-13 December 2000.
 9. D. Ridikas et al., “Comparative Analysis of ENDF, JEF and JENDL Data Libraries by Modelling High Temperature Reactors and Plutonium Based Fuel Cycles: Military Pu case”, *Proceedings of the Int. Conference on Nuclear Data for Science and Technology (ND2001)*, Tsukuba, Japan, 7-12 October 2001.
 10. D. Ridikas et al., “Comparative Analysis of Different Data Libraries for the Performance of High Temperature Reactors (GT-MHR): Civil Pu case”, *Proceedings of the Int. Conference on Accelerator Applications/Accelerator Driven Transmutation Technology and Applications (AccApp/ADTTA'01)*, 12-15 November 2001, Reno, Nevada, USA.