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Feasibility of Weak Irradiation in the HFR as a Tool for Pre-Irradiation Qualification of HTR Fuel

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A conceptual design for such an installation was prepared. Neutron metrology in combination with neutronic calculations enabled determining the locally achievable thermal neutron fluxes in the newly configured HFR core with LEU fuel. With these neutron fluxes as input, the required exposure times to detect characteristic fission gas R/B fractions (release over birth) of 10^{-5} from Xe-135 were estimated to be 16 days for a single pebble (AVR type). Although sensitivities of R/B = 10^{-8} are reported in literature, the achieved sensitivity would mean that it is possible to detect a single leaking particle in a pebble from which 10% of the fission gas production is escaping.

Future work is outlined including the required financial investment for making such an installation operational. In particular due to the expected mismatch between potential benefit (number of future customers) and available resources at JRC-IE, no decision could currently be taken in favor of construction and testing of such an installation.

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Feasibility of Weak Irradiation in the HFR as a Tool for Pre-Irradiation Qualification of HTR Fuel

Deliverable RAPHAEL-0610-D-FT1.3
for the RAPHAEL Integrated Project

rev. A

Michael A. Fütterer, Alain Marmier, Josselin Morand,
Lango Metten, Alan van de Sande

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This report provides a feasibility assessment of weak irradiation tests in the horizontal neutron beam HB8 of the HFR Petten.

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1 Introduction

In the FP6 RAPHAEL Integrated Project which started in April 2005 for a duration of 4 years, 7 of the 33 partner organizations work together to recover the full know-how of HTR fuel fabrication originally developed in Germany and to further improve the produced fuel. The fuel may come in the shape of spherical fuel elements ("pebbles") or cylindrical sticks ("compacts"). New fuel types and coating techniques are under development and will ultimately require testing under normal irradiation conditions and simulated accidental conditions. These irradiation tests, which are a licensing requirement, are expensive and time consuming (typical project duration 3 – 5 years) so that there is an incentive to make sure that only sufficiently qualified fuel is actually irradiated. Furthermore, it would be instructive to benchmark the non-destructive weak irradiation method against the destructive and time-consuming leach-burn-leach method for determining particle failure fractions of as-received fuel.

This document describes work performed so far on the weak irradiation method including neutron flux measurements, irradiation requirements, design options and the construction of a new shielding for the horizontal neutron beam HB8 in the HFR Petten (Figures 1 and 2). Finally, the remaining work is described and estimates for additional expenditure are given which would be required to make this method fully operational.

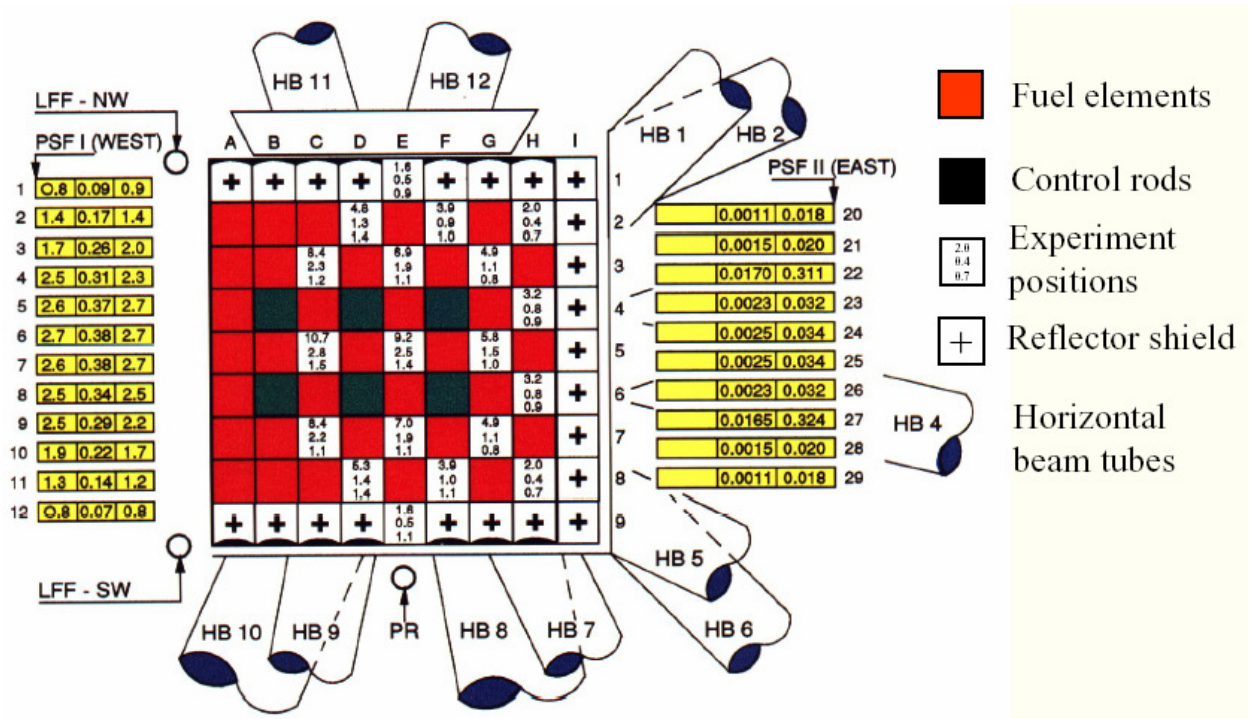

Figure 1: HFR core layout and neutron beam arrangement

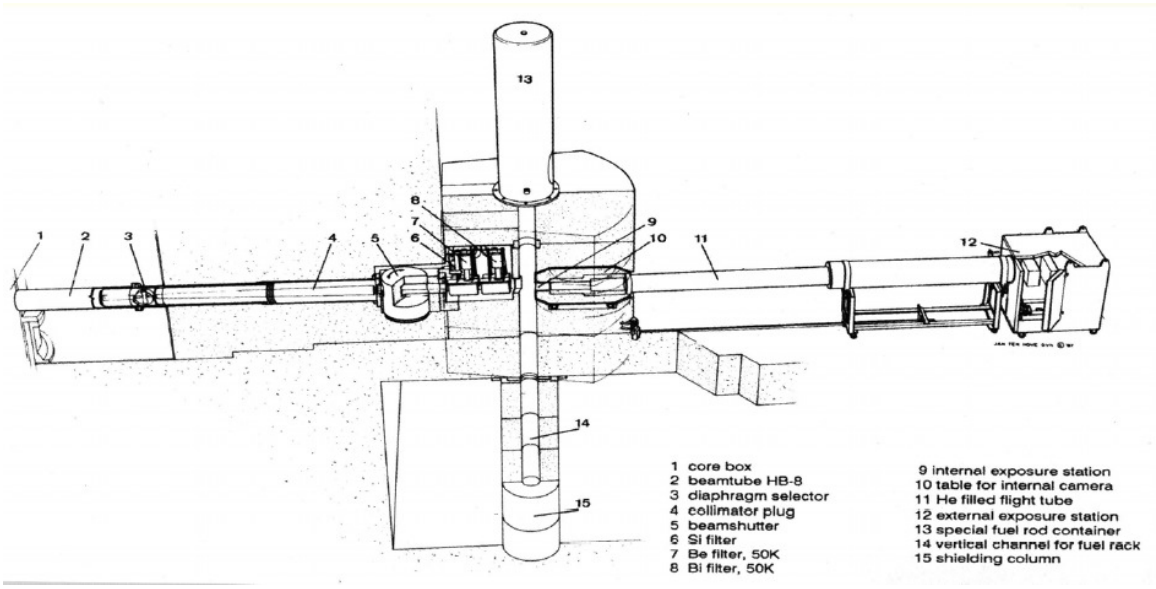

Figure 2: Horizontal beam tube HB8 in the HFR Petten, usually employed for neutron radiography

2 Requirements

Among others, General Atomics had in the past performed weak irradiation testing on HTR fuel compacts. These compacts (comprising of some 5000 fuel particles) underwent approx. 7.45×10^{13} fissions per compact at 1100°C in a TRIGA reactor which enabled the detection of R/B = 1.6×10^{-8} for Kr-85m. The flux is unknown and the duration of irradiation was of the order of hours.

To determine the feasibility of weak irradiation in the HFR, two possible approaches could be used:

1. Target the same number of fissions as those for General Atomics compacts.
2. Using the sensitivity of gamma spectrometry equipment to conclude on required radioactivity concentration in purge gas. For a typical R/B value at BOI, then calculate number of fissions required and exposure time.

As a constraint, the fuel activity after irradiation had to be limited such that it can still be handled immediately after weak irradiation without particular precautions, e.g. to enable the manual assembly of the fuel in a dedicated irradiation rig. A neutronic model was required taking due account of shielding needs, real geometry and absorption effects.

The duration of the exposure should be as short as possible so that weak irradiation testing of fuel could be used in a routine manner.

2.1 Neutron metrology

The achievable thermal neutron flux is a decisive input for determining the feasibility of weak irradiation. Due to the conversion of the HFR from high-enriched uranium to low-enriched uranium, which was completed in May 2006, the neutron fluence in HB8 was reassessed. For this purpose, activation monitor sets were placed into the neutron beam at constant reactor power and were activated. The duration of exposure was approximately 3 hours. From the activation analysis, the thermal neutron flux could be deduced [1], [2].

The monitor sets contained foil disks of three different materials:

- AuAl 1 wt% Au, thickness = 0.2 mm, ∅ = 20 mm
- Cu 100 wt% Cu, thickness = 0.1 mm, ∅ = 20 mm
- MnNi 88 wt% Mn, thickness = 0.1 mm, ∅ = 20 mm

The following reactions were used for neutron metrology:

- Au-197 (n,γ) Au-198
- Cu-63 (n,γ) Cu-64
- Mn-55 (n,γ) Mn-56

The activities of the foils were counted at calibrated distances of a high purity Germanium (HPGe) detector coupled to an 8192 channel pulse amplitude analyzer. Knowing the duration of foil exposure, the reaction rates of the Au, Cu and Mn reactions were determined (Table 2). Using a custom-made MCNP model for neutron beam and the foils as the target, the thermal neutron flux was adjusted as a parameter to reach the measured reaction rates. This was the way the thermal flux was recalculated. From the obtained

thermal flux, a fission rate per pebble, placed at the centre of the beam exit, was deduced to be approximately 5.03×10^5 fissions/s. The calculation scheme for the related neutronic calculations is detailed in section 8. Only the filter combination in Case 2 was found useful because all other combinations led either to lower neutron fluxes or to increased neutron scattering and gamma emission. Calculations for compacts have not been performed yet. In the current set-up of the HB8 environment, operation without filters has not yet been possible due to excessive gamma dose rates in the neighboring working area. Once the new shielding is installed, this measurement will be attempted again.

Location	Filters	Reaction rates [$s^{-1}at^{-1}$]	Fission Rate in Pebble [fissions/s]
1. center of beam, 55 cm from beam exit	Be + Bi cooled	Au: 6.656E-17 Cu: 2.951E-18 Mn: 8.364E-18	N/A
2. center of beam, at beam exit	Be + Bi cooled	Au: 7.975E-17 Cu: 3.573E-18 Mn: 1.020E-17	5.03×10^5
3. center of beam, at beam exit	Si + Pb uncooled	Au: 8.596E-18 Cu: 3.904E-19 Mn: 1.082E-18	N/A
4. center of beam, at beam exit	Pb uncooled	Au: 1.988E-17 Cu: 8.572E-19 Mn: 2.362E-18	N/A
5. center of beam, at beam exit	Bi cooled	Au: 8.550E-17 Cu: 3.885E-18 Mn: 1.104E-17	N/A

Table 1: Neutron metrology results for HB8 at different locations and with different filter combinations

Note that the 55 cm layer of air between the beam exit and the probable target location in the external exposure station, cf. Figure 2 cause a flux depression of approx. 18%. Due account of this was taken in the neutronic model. As mentioned above, the type and combination of filters also has significant influence on the flux.

2.2 Estimated duration of neutron exposure

Using the fission rate as determined from neutron metrology, the required exposure time could be estimated. This exposure time should be as short as possible to enable in series testing of fuel specimens. The approach was to use the sensitivity of the fission gas detectors to determine the duration.

As targets any type of HTR fuel can be used, e.g. pebbles or compacts. Typical values used in our estimations are:

	Compact (General Atomics)	Pebble (AVR)
Diameter [mm]	12.5	60
Length [mm]	50	N/A
Number of particles	5035	9560
Total U content [g]	3.42	6
U-235 content [g]	0.36	1

Table 2: Assumed characteristics of fuel targets

Calculated from instrument sensitivity			
Fission rate	5.03×10^{5} fissions/s (lower estimate)		
Fission yield	Kr-88	Xe-135	
	3.47×10^{-2}	6.58×10^{-2}	
Sensitivity of gamma spectrometry (HP Ge detector):	$\approx 7.3\times10^{5}$ at (50 Bq)	$\approx 4.6\times10^{5}$ at (10 Bq)	
Lower R/B limit to be detectable:	10^{-7}	10^{-6}	10^{-5}
Required conditions for detection of Xe-135:			
Required number of fissions	6.99×10^{13}	6.99×10^{12}	6.99×10^{11}
Exposure time for a single pebble	1690	160.9	16.1
Required conditions for detection of Kr-88:			
Required number of fissions	1.44×10^{15}	1.44×10^{14}	1.44×10^{13}
Exposure time for a single pebble	3316	331.6	33.2

Table 3: Estimated required exposure time for weak irradiation of an AVR pebble

The product *fission yield* × *detection sensitivity* is larger for Xe-135, so that a shorter irradiation time is required for this isotope, which was therefore chosen as the reference.

This means that:

- The required irradiation time is quite long: only one or two pebbles can be tested within a single HFR cycle (28 days);

- The realistically achievable sensitivity of this method is rather low (detectable R/B ≈ 10^{-5}) but possibly acceptable as this value would correspond to the ability to detect a single leaking particle that releases 10% of its fission gas production.

3 Conceptual Design of Weak Irradiation Facility

The basic idea was to place the fuel to be tested in a gas-tight cylindrical metal container and to expose this container to a known neutron flux. Several neutron beams and other facilities in the HFR exist with various achievable neutron fluxes. The horizontal beam tube HB8 was selected as it features one of the highest neutron fluxes and would have been available for such installations. The irradiation should be performed at nominal fuel temperature to accelerate possible fission gas transport to the steel container. This requires a heater and suitable ventilation of the shielding box. The entire installation requires shielding to protect operators as HB8 is situated in a rather busy passage area on the HFR ground floor. The shielding of HB8 was completely refurbished (cf. Figure 3), installation of the new equipment is in progress [4].

Figure 3: New shielding box for HB8

In principle, two approaches can be used to determine the R/B value from weak irradiation:

1. **Stagnant gas in container, fission gas accumulation:** In this case, the container is pressurized with He to 1.2 bar at room temperature (= 6 bar at 1200°C). This should be the limit because the container bottom should remain as thin and neutron transparent as possible. After irradiation, the gas containing the volatile fission products is transferred to a standard gas-sampling vessel like those used in other irradiation tests. Although released volatile fission gases are not expected to adsorb on graphite during cool-down, the cover gas in the container can be transferred via long minitubes to the (evacuated) gas-sampling vessel on the outside of the shielding box while the irradiated sample (fuel) is still hot. This standard gas-sampling vessel is then placed on an external HP Ge detector (gamma spectrometry) with a multi-channel analyzer calibrated for this purpose.

2. **Active gas purging:** The steel container can be connected to a gas system supplying a low controlled flow-rate of He (e.g. 1 ml/min) at controlled pressure for on-line measurement of fission gas concentrations in the purge gas by NaI detectors (gamma spectrometry). This would enable the deduction of the characteristic R/B value. However, as the fuel is continuously purged, the sensitivity of the NaI detector would need to be much higher than that of the HP Ge detector to detect the same R/B. Therefore, we have discarded this method from our considerations.

A conceptual design of a container is shown in Figure 4 and its implantation into the shielding box is displayed in Figure 5.

Similarly to in-pile irradiation tests, the fuel targets to be irradiated will be packed into graphite cylinders to ensure good heat transfer from the external heater to the fuel. The target temperature will be monitored using at least one type N thermocouple. These thermocouples can also be used to automatically control the temperature by adjusting the heater power. A fission gas volume of several cm^3 is foreseen to accumulate in the container. The container is sealed with a lid and a metal gasket. A suitable gasket type (conical or S shape) will need to be found experimentally to guarantee leak tightness during the thermal cycling from room temperature to operating temperature and back. Alternatively, the lid could be welded such that both container and lid can be re-used. The lid facing the beam tube has to be thick enough to tolerate an operating pressure of approx. 6 bar at high temperature but thin enough to not significantly absorb neutrons. The backside of the container is equipped with passages for thermocouples that are sealed leak tight by high temperature brazing. The bottom is also connected to two minitubes with sufficient length (approx. 1 m) to reach out of the shielding box. A snap-tight gas connector (Stäubli type) is welded to each minitube to enable connection to a gas circuit. The temperature of the gas-sampling container will equally be measured. Purging at approx. 150°C is required for at least 24 h to drive out moisture from graphite and fuel.

Suitable materials for this container would be a zirconium alloy (melting point of 1850°C) or niobium (melting point of 2470°C) as they are compatible with high temperatures and are rather transparent for thermal neutrons.

The heating could be provided either by externally insulated heating elements brazed to the walls of the container or by placing the container into a cylindrical furnace which is used for material testing. While these furnaces are able to reach central temperatures of approx. 1600°C the container will need to be positioned at the furnace extremity to enable capturing a maximum of the neutron flux. The achievable temperatures in the end part of such a furnace will need to be measured experimentally before opting for one or another solution.

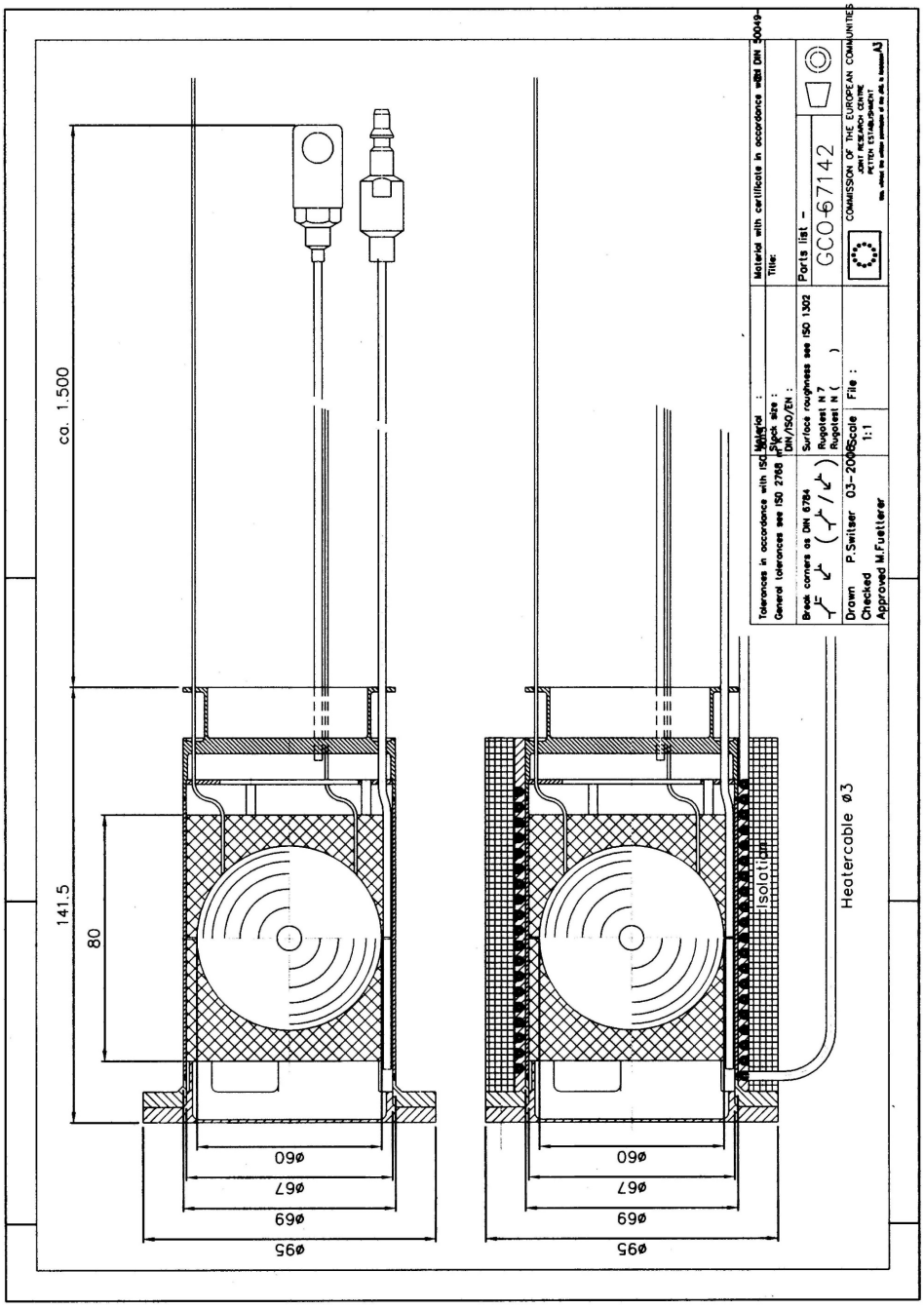

Figure 4: Conceptual design of an irradiation container with and without heating elements

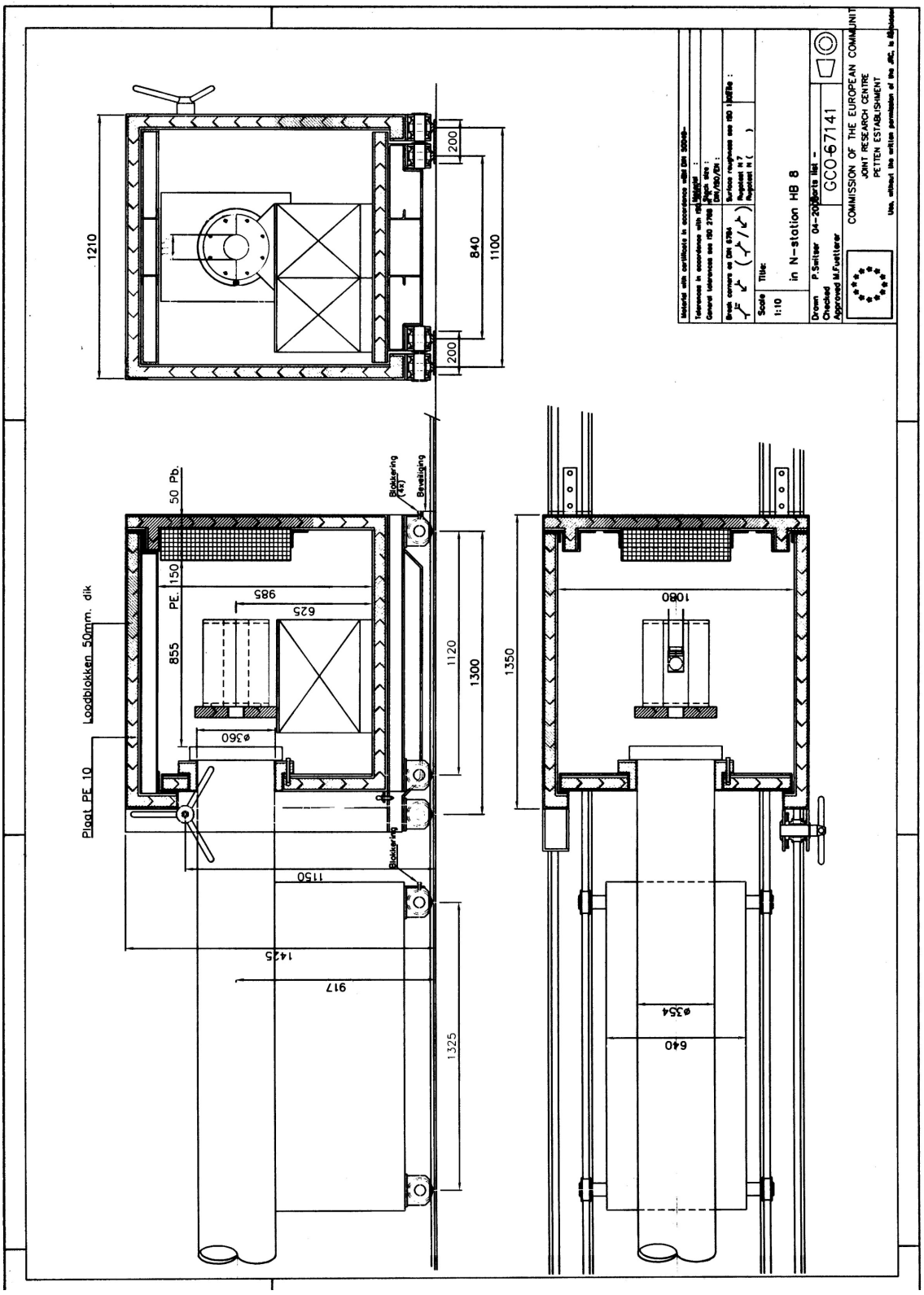

Figure 5: HB8 with shielding box and irradiation container

4 Gas Circuit

The function of this gas circuit is to supply vacuum and He for purging at controlled flow rate and pressure, and to transfer the accumulated fission gas to the gas-sampling container by pressure equilibration. The circuit has to be mounted on a panel within a glove box in the vicinity of HB8 and requires a connection to the HFR He supply and off-gas system. For safety reasons, radioactivity monitoring will be required.

A conceptual design of this gas circuit is shown in Figure 6

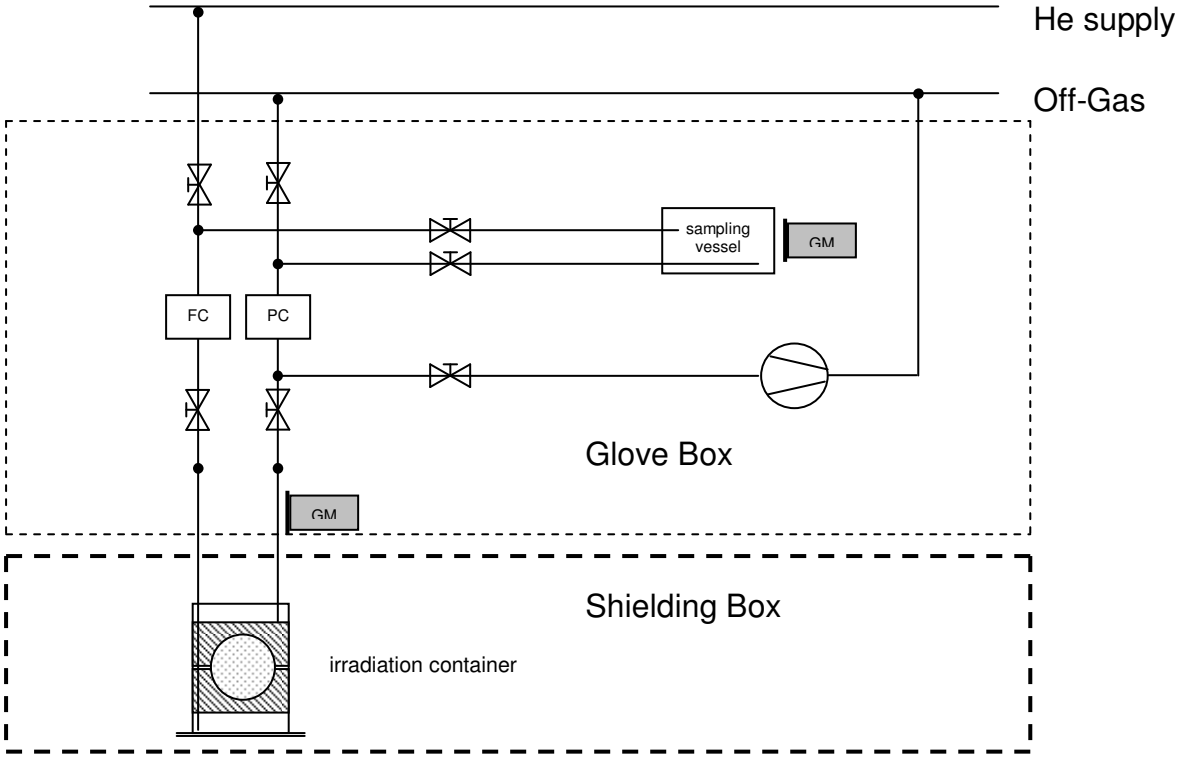

Figure 6: Conceptual design of a gas circuit

5 Additional Required Work and Expenditure

The following list provides the further required work to make this method operational in the HFR and an estimate for budget requirements.

Item	Cost Estimate [k€]
Manufacturing of graphite and metal parts	5
Experimental determination of high temperature brazing parameters	3
Connection to He supply and HFR off-gas system	1
Glove box	2
Ventilation of shielded box	3
Gas analysis for 10 trials (existing)	3
Experimental determination of suitable seal	3
Construction of a gas circuit	5
Choice of heating system	1
Furnace	6
Design and Safety Report	7
Total	**38**

6 Conclusions

The main result of this feasibility study is that, in principle, weak irradiation of HTR fuel is possible in the neutron beam HB8 of the HFR. Several alternatives for HB8 are still under investigation to possibly increase the achievable neutron flux. In HB8, The required irradiation time is quite long: only one or two pebbles can be tested per one HFR cycle (28 days) and the realistically achievable sensitivity of this method is relatively low (realistic minimum detectable R/B $\approx 10^{-5}$). This value is possibly acceptable, as it would correspond to the ability to detect a single leaking particle in a pebble that releases 10% of the fission gases produced there.

Weak irradiation as a routine test of HTR fuel prior to in-core irradiation would have a non-negligible impact on the schedule of an irradiation project (+2.5 months for an irradiation of typically 5 pebbles and +10 months for an irradiation of typically 10 compacts).

Considering the limited effort on fuel fabrication in Europe, the potential number of candidate specimens for this type of test in the next few years is fairly low.

Opponents of weak irradiation tests claim that they proved little useful in the past as even successfully tested fuel specimens could fail after a short period of irradiation.

Furthermore, the required financial and manpower effort to demonstrate weak irradiation in the HFR is not in a reasonable relation to the expected benefit and the budget provided by RAPHAEL. This mismatch is the reason why JRC-IE has decided, at this point, to not go ahead with the construction and testing of such a facility.

7 References

[1] A. Paardekooper, Neutron fluence rate measurement in HB8, NRG Note 911635/06.74732/MMI/AP/MH, 14 July 2006.

[2] A. Paardekooper, Neutron fluence rate measurement in HB8, NRG Note 911668/06.75714/MMI/AP/LRD, 1 September 2006.

[3] J. Ahlf, A. Zurita, ed., High Flux Reactor (HFR) Petten – Characteristics of the Installation and the Irradiation Facilities, Commission of the European Communities, EUR 15151 EN, 1993.

[4] L. Metten, A. van de Sande, F. Klaassen, K. Bakker, A. Bontenbal, The HFR HB8 neutron radiography facility, Proc. 8th World Conference on Neutron Radiography WCNR-8, Gaithersburg, MD, USA, 16-19 October 2006.

8 Annex: MCNP Neutronic Calculations

MCNP simulations require an energy spectrum and directional distribution of incident neutrons. As MCNP results are normalized per emitted/source neutron intensity (an MCNP calculated neutron flux over a surface will be in $n * cm^{-2} * n_{emited}^{-1}$), the intensity will be required only when absolute values of e.g. reaction rates or fluxes are to be determined.

Several aspects are important in case of an MCNP calculation. Amongst the most important are model geometry, material and source definitions

For this project, pebbles were already defined for a study related to the HFR-EU1bis irradiation test. The surrounding was slightly modified to match the real experimental design. Neutron flux measurements from the former high enriched uranium core and the new low enriched uranium core of the HFR allowed reconstructing neutron flux in HB8.

The neutron beam flux was measured and compared between the high enriched and low enriched uranium core of the HFR. This allowed the reconstruction of neutron flux and spectrum which was then used as input for the simulations with the fuel pebble to be irradiated.

8.1 Source reconstruction

8.1.1 Data

Monitor	Mass (mg)	Activity (Bq)	Uncertainty (%)	Reaction rate (s^{-1})	Ratio LEU/HEU
AuAl 2	171.05	1.090E+01	1.79	6.656E-17	1.0238
Cu 2	285.92	8.277E+02	1.67	2.951E-18	1.0200
MnNi 2	226.22	1.004E+04	0.61	8.364E-18	1.0127
AuAl 3	174.87	1.369E+01	1.83	7.975E-17	----
Cu 3	286.06	1.026E+03	0.69	3.573E-18	----
MnNi 3	223.72	1.231E+04	0.53	1.020E-17	----

Table 7: Foils mass values, activities and reaction rates

Monitor set	Spectrum indices			ϕ_0	uncertainty	θ	uncertainty
	Au/Mn	Au/Cu	Mn/Cu	($m^{-2}.s^{-1}$)	(%)	($m^{-2}.s^{-1}.u^{-1}$)	(%)
2	7.96	22.6	2.83	6.48E+09	2.6	1.54E+07	87
3	7.82	22.3	2.85	7.88E+09	2.2	1.13E+07	135

Table 8: Fluence rates/neutron fluxes for thermal and intermediate spectra (Φ_0 and Θ, respectively). The reactor power was 45 MWth.

Monitor set	Start	Stop	Remarks
2	20060628 091152	20060628 121005	Position of film in the centre of the beam 55cm from beam exit.
3	20060628 121455	20060628 151744	At the end of the beam in the centre of the beam

Table 9: Irradiation histories

These results were obtained by irradiation of three different foils placed at the HB8 exit. After irradiation, activities measured allowed to reconstruct the neutron flux in the position of the foils. Unfortunately, flux "seen" by the foils is not the flux emitted by HB8 as neutrons might diverge between HB8 exit and the foils.

To properly determine the intensity of source neutrons (normalization factor), the first calculation performed with MCNP was to simulate the irradiation of a foil (copper) used for experimental flux determination using the determined value of the thermal source flux. As an approximation, taking into account HB8 geometry, the directional distribution of source neutrons was assumed to parallel with the beam axis. This approach may somewhat overestimate the value of the normalization factor.

8.1.2 Copper foil for normalization factor determination

As mentioned above, the irradiation of the copper foil was simulated. Indeed, out of the three foils used in the experiment (AuAl, Cu, MnNi), the copper foil proved to be the most sensitive to thermal neutrons (however, AuAl foils have consistently the highest reaction rates and spectral indices). The aforementioned conclusion was reached by comparing MCNP reaction rates of the three foils using neutron flux with the Maxwellian part of the energy spectra only as a source. The latter approach also considerably simplified the source design.

Below is the MCNP input file required for the calculation of the normalization factor ($neutron\_emitted * s^{-1}$). The measured and calculated reaction rates of Cu-63 (n, γ) Cu-64 have to be compared.

Copper Foil with HB8 source

1 1 -8.92 3 -4 -2 imp:n=1 imp:n=1 $ Foil

2 0 -1 #(3 -4 -2) imp:n=1 imp:n=1 $ Void with importance

3 0 1 imp:n=0 imp:n=0 $ Univers limit

1 so 80 $ Importance border

2 pz 0.005 $ Foil border

3 pz -0.005 $ Foil border

4 cz 1.0 $ Foil border

5 pz -55.005 $ Source

SDEF SUR 5 POS 0 0 -55.005 RAD D1 DIR 1 VEC 0 0 1 NRM 1 PAR 1 ERG D2 $ Source

SI1 3.35 $ Diameter boundary

SP1 -21 1 *$ Sample on diameter*
SI2 L 0 .563E-6 *$ Energy Boundaries*
SP2 -5 0.025E-6 *$ Maxwellian function*
F4:n 1 *$ Flux of neutrons over the foil*
FM4 5.96590E-02 *2 102* *$ Reactions rate Cu63(n,Gamma)Cu64*
NPS 15E6 *$ 5E6 Neutrons shot*
PRINT *$ Print*
m1 29000 1. *$ Natural copper*
m2 29063 1. *$ Isotope 63 copper*

Copper Foil with HB8 source
1 1 -8.92 3 -4 -2 *imp:n=1 imp:p=1* *$ Foil*
2 0 -1 #(3 -4 -2) *imp:n=1 imp:p=1* *$ Void with importance*
3 0 1 *imp:n=0 imp:p=0* *$ Univers limit*

1 so 80 *$ Importance border*
2 pz 0.005 *$ Foil border*
3 pz -0.005 *$ Foil border*
4 cz 1.0 *$ Foil border*
5 pz -55.005 *$ Source*

Tally F4 with multiplier FM4 calculates the (n, γ) reaction rate of the material m2 over the cell per neutron emitted per volume. The multiplier FM4 takes into account Cu-63 atomic density: The foil is made of 285.92 mg of natural copper thus only 63.3% of its weight is Cu-63, leading to an atomic density of $5.9659 * 10^{-2} atom * (barn * cm)^{-1}$.

1tally 4 nps = 15000000
tally type 4 track length estimate of particle flux.
tally for neutrons

volumes
cell: 1
3.14159E-02

cell 1
multiplier bin: 5.96590E-02 2 102

6.94315E-03 0.0011

Multiplication of tally 4 by the foil volume gives the reaction rate over the foil per incident neutron. As the measured reaction rate is known, dividing this value by the calculated one gives the neutron intensity to be emitted (normalization factor) to reach the right foil activation.

$$Calculated\_(n,\gamma)\_reaction\_rate = T_4 * V_f$$

With T_4 reaction rate per neutron emitted per volume and V_f the foil volume: $T_4 = 6.94 * 10^{-3} (n,\gamma)\_reaction * cm^{-3} * neutron\_emitted^{-1}$ and $V_f = 3.14 * 10^{-2} cm^3$

$$Calculated\_(n,\gamma)\_reaction\_rate = 2.18 * 10^{-4} (n,\gamma)\_reaction * neutron\_emitted^{-1}$$

At the position 55 cm from the beam exit, the measured reaction rate is $2.95 * 10^{-18} (n,\gamma)\_reaction * \mathrm{s}^{-1} * Cu_{63\,atom}$. Taking the copper foil mass into account, amount of Cu-63 atoms can be estimated as being $1.87 * 10^{21}$, leading to a foil reaction rate of $5.53 * 10^{3} (n,\gamma)\_reaction * \mathrm{s}^{-1}$.

This yields a normalization factor $NF = 2.54 * 10^{7} * neutron\_emitted * s^{-1}$ which will serve for the normalization of our next MCNP results. Using this normalization factor, a calculated thermal flux in HB8 was then determined to be $\Phi_{HB8} = 7.19 * 10^{5} n * s^{-1} * cm^{-2} = 7.19 * 10^{9} n * s^{-1} * m^{-2}$. The neutrons were sampled over a surface perpendicular to the beam axis located on the beam exit, its surface being 35.25 cm^2.

8.2 Pebble and experiment model

The same neutron source was then applied for a simulation of the pebble irradiation in the capsule. Three different pebble models were built: a pebble with mixed composition of kernel and carbon matrix (homogenous mixture), a pebble with coated particles in a regular lattice arrangement, and finally a pebble composed of 9560 coated particles randomly distributed within the graphite matrix.

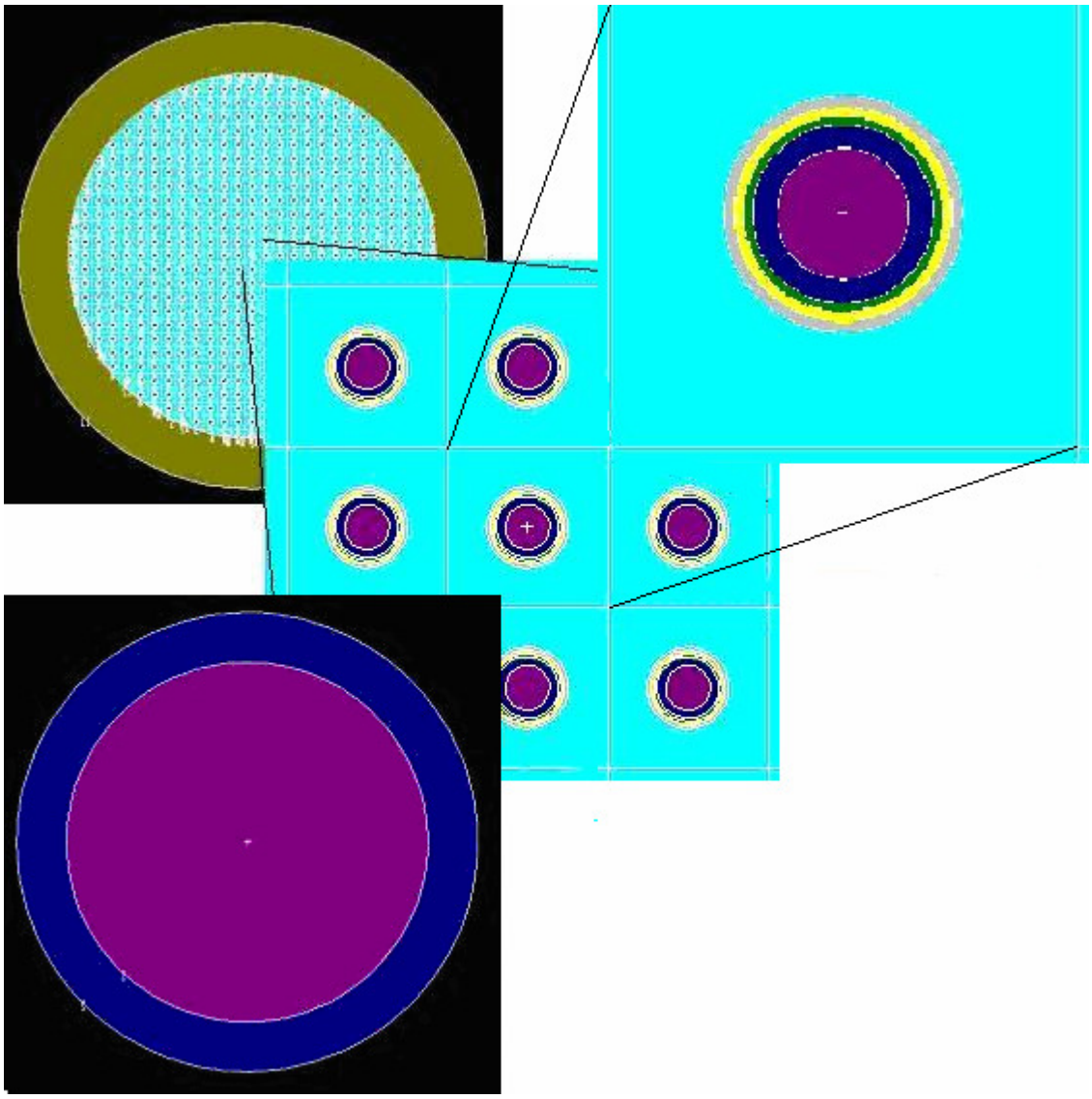

Figure 7: A pebble with coated particles in a regular lattice arrangement

8.2.1 Homogenous pebble

Below is the MCNP input file required for the abovementioned simulation:

Pebble with Homogenous kernel and HB8 as source

1 1 -1.87 -1 TMP=1.2926-7 imp:n=1

2 2 -1.75 1 -2 TMP=1.2926-7 imp:n=1

3 2 -1.75 (-3 4 -5) #(-2) TMP=1.2926-7 imp:n=1

4 3 -8.57 (-3 6 -4) TMP=1.2926-7 imp:n=1

5 0 (3:-6:5) -7 TMP=1.2926-7 imp:n=1

6 0 7 imp:n=0

1 so 2.35

```
2 so  3.0
3 cz  3.35
4 pz -4.0
5 pz  4.0
6 pz -4.1
7 so  80
8 pz -29.1

SDEF SUR 8 POS 0 0 -29.1 RAD D1 VEC 0 0 1 DIR 1 AXS 0 0 1 NRM 1 PAR 1 ERG D2
$ Source
SI1 3.35                                        $ Diameter boundary
SP1 -21 1                                        $ Sample on diameter
SI2 L 0 .563E-6                                   $ Energy Boundaries
SP2 -5 0.025E-6                                    $ Maxwellian function
F4:N 1
F14:N 1
FM14 -1 1 -6
NPS 15E6
PRINT
m1   6000  -0.93155  8016  -0.00812  14000 -3.196E-5
     92235 -0.999-2  92238 -0.05030
m2   6000  1.
m3   41093 1.
```

8.2.2 Lattice pebble

Below is the MCNP input file required for this simulation:

```
Pebble with heterogeneous kernel and HB8 as source
1   1  -10.97       -1              TMP=1.2926-7 u=1 imp:n=1
2   2  -1.02        1 -2            TMP=1.2926-7 u=1 imp:n=1
3   3  -1.92        2 -3            TMP=1.2926-7 u=1 imp:n=1
4   4  -3.2         3 -4            TMP=1.2926-7 u=1 imp:n=1
5   5  -1.92        4 -5            TMP=1.2926-7 u=1 imp:n=1
6   6  -1.75        5               TMP=1.2926-7 u=1 imp:n=1
7   0             -6 7 -8 9 -10 11     lat=1 fill=1 u=2 imp:n=1
```

```
8   0            -12                  fill=2     imp:n=1
9   7  -1.75       12 -13             TMP=1.2926-7     imp:n=1
10  7  -1.75       (-14 15 -16) #(-13) TMP=1.2926-7     imp:n=1
11  8  -8.57       (-14 -15 17)       TMP=1.2926-7     imp:n=1
12  0            (14:-17:16) -19                imp:n=1
13  0            19                           imp:n=0

1  so  .02505
2  so  .03425
3  so  .03755
4  so  .04125
5  so  .0455
6  pz  .0892445
7  pz -.0892445
8  px  .0892445
9  px -.0892445
10 py  .0892445
11 py -.0892445
12 so  2.35
13 so  3.0
14 cz  3.35
15 pz -4.0
16 pz  4.0
17 pz -4.1
18 pz -29.1
19 so  80

SDEF SUR 18 POS 0 0 -29.1 RAD D1 VEC 0 0 1 DIR 1 AXS 0 0 1 NRM 1 PAR 1 ERG D2
SI1 3.35
SP1 -21 1
SI2 L 0 .563E-6
SP2 -5 0.025E-6
m1   8016 -.11872 92235 -.14606 92238 -.73522
m2   6000 1.
m3   6000 1.
```

```
m4   6000 12.01   14000 28.06
m5   6000 1.
m6   6000 1.
m7   6000 1.
m8   41093 1.
m9   6000 -0.93155  8016  -0.00812  14000 -3.196E-5
     92235 -0.999-2  92238 -0.05030
F4:N 8
F14:N 8
FM14 8.61528E-02 9 -6
F24:N 8
FM24 -1 9 -6
F34:N 1
F44:N 1
FM44 -1 1 -6
F54:N (1<7[0 0 0])
F64:N (1<7[0 0 0])
FM64 -1 1 -6
NPS 15E6
Print
```

8.2.3 Randomly generated pebble

Due to the size of the input file, only the method will be described here: Based on a Visual Basic code, the 9560 particles were randomly distributed in the pebble. Then, the code automatically generates the input file for the simulation by translation of this coated particle to the defined positions.

8.3 Results

8.3.1 Homogenous pebble

Tally 4 measures the neutron flux per emitted neutron over cell 1 (the inner part of the pebble composed of a mixture of kernels and carbon matrix).

1tally 4 nps = 15000000
*tally type 4 track length estimate of particle flux. units 1/cm**2*
tally for neutrons

volumes

cell: 1

5.43616E+01

cell 1

2.08845E-02 0.0005

$T_4 = 2.08845 * 10^{-2} \mathrm{n} * \mathrm{cm}^{-2} * neutron\_emitted^{-1}$

This leads to a neutron flux over the whole pebble of $\Phi_{C1} = T_4 * NF$

$\Phi_{C1HO} = 5.30 * 10^5 n * cm^{-2} * s^{-1}$

Tally 14 measures the fission rate per volume per emitted neutron over the whole pebble.

1tally 14 nps = 15000000

tally type 4 track length estimate of particle flux.

tally for neutrons

volumes

cell: 1

5.43616E+01

cell 1

multiplier bin: -1.00000E+00 1 -6

3.22104E-04 0.0006

$T_{14} = 3.22104 * 10^{-4} \mathrm{fission} * cm^{-3} * neutron\_emitted^{-1}$

Cell 1 volume is $V_{C1} = 54.36 cm^3$

This leads to a fission rate over cell1 of $FR_{HO} = T_{14} * V_{C1} * NF$

$FR_{HO} = 4.44 * 10^5 \, fission * s^{-1}$

8.3.2 Lattice pebble

Tally 4 measures the neutron flux per emitted neutron over cell 8 (the inner part of the pebble composed of the carbon matrix with 9560 coated particles).

1tally 4 nps = 15000000
tally type 4 track length estimate of particle flux. units 1/cm**2
tally for neutrons

volumes
cell: 8
5.43616E+01

cell 8
2.07970E-02 0.0005

$T_4 = 2.0797 * 10^{-2} \mathrm{n} * cm^{-2} * neutron\_emitted^{-1}$

This leads to a flux over cell 8 of $\Phi_{C8HE} = T_4 * NF$: $\Phi_{C8HE} = 5.28 * 10^5 n * cm^{-2} * s^{-1}$

Tallies 14 and 24 and their multipliers measure the fission rate over cell 8 per volume per emitted neutron. Here, the neutron transport is made with the regular lattice structure, but the tally is calculated as in the homogenous approach. In the first case (tally 14), the atomic density is specified, in the second (tally 24), MCNP has to calculate it on its own.

1tally 14 nps = 15000000
tally type 4 track length estimate of particle flux.
tally for neutrons

volumes
cell: 8
5.43616E+01

cell 8
multiplier bin: 8.61528E-02 9 -6

3.17937E-04 0.0006

$T_{14} = 3.17937 * 10^{-4} \text{fission} * cm^{-3} * neutron\_emitted^{-1}$

Cell 8 volume is $V_{C8} = 54.36 cm^3$

This leads to a fission rate over cell 8 of $FR_{C8\,HET14} = T_{14} * V_{C8} * NF$:
$FR_{C8\,HET14} = 4.38 * 10^5 \; fission * s^{-1}$

1tally 24 nps = 15000000
tally type 4 track length estimate of particle flux.
tally for neutrons

volumes
cell: 8
5.43616E+01

cell 8
multiplier bin: -1.00000E+00 9 -6
3.21806E-04 0.0006

$T_{24} = 3.21806 * 10^{-4} \text{fission} * cm^{-3} * neutron\_emitted^{-1}$

Cell 8 volume is $V_{C8} = 54.36 cm^3$

This leads to a fission rate over cell 8 of $FR_{C8\,HET24} = T_{24} * V_{C8} * NF$:
$FR_{C8\,HET24} = 4.43 * 10^5 \; fission * s^{-1}$

Tally 34 measures the neutron flux over cell 1 per emitted neutron. Here the tally applies to the inner part of the kernel (UO_2) that will be duplicated in the regular lattice structure. Therefore, it actually represents an integral over all kernels.

1tally 34 nps = 15000000
tally type 4 track length estimate of particle flux. units 1/cm**2
tally for neutrons

volumes

cell: 1

6.58433E-05

cell 1

1.90937E+02 0.0009

$T_{34} = 1.90937 * 10^{2}\,\mathrm{n} * cm^{-2} * neutron\_emitted^{-1}$

This leads to an averaged flux over all kernels (UO_2 part of the kernel) of $\Phi_{C9560KHE} = T_{34} * NF$

$\Phi_{C9560KHE} = 4.82 * 10^{9} n * cm^{-2} * s^{-1}$

For one particle, this result should be divided by the total amount of particles: 9560

$\Phi_{C1KAHE} = T_{34} * NF / 9560$

$\Phi_{C1KAHE} = 5.04 * 10^{5} n * cm^{-2} * s^{-1}$

Tally 44 and its multiplier measures the fission rate over cell 1 per volume per emitted neutron. Here the tally applies to the inner part of the kernel, thus the material is the enriched UO_2. Again, as cell 1 will be duplicated in the lattice structure, it actually represents an integral over all kernels.

1tally 44 nps = 15000000

tally type 4 track length estimate of particle flux.

tally for neutrons

volumes

cell: 1

6.58433E-05

cell 1

multiplier bin: -1.00000E+00 1 -6

2.32114E+02 0.0010

$T_{44} = 2.32114 * 10^{2}\,\mathrm{fission} * cm^{-3} * neutron\_emitted^{-1}$

Cell 1 volume is $V_{C1} = 6.58433 * 10^{-5} cm^3$

This leads to an integral fission rate in the pebble of $FR_{C9560K\,HE} = T_{44} * V_{C1} * NF$

$FR_{C9560K\,HE} = 3.87 * 10^5 \; fission * s^{-1}$

We are interested in the total fission rate in the pebble. Therefore tallies 34 and 44 were applied to the cell that is duplicated into the regular lattice. Indeed, this cell collects the flux in each particle/kernel. Then volume normalization in tally 44 should be done for one particle only.

Tally 54 measures the neutron flux per emitted neutron over the kernel of one particle/kernel, precisely the one lying in the center of the pebble.

1tally 54 nps = 15000000
tally type 4 track length estimate of particle flux. units 1/cm**2
tally for neutrons

volumes
cell: 1
6.58433E-05

cell (1<7[0 0 0])
2.04369E-02 0.0439

$T_{54} = 2.04369 * 10^{-2} \, \mathrm{n} * cm^{-2} * neutron\_emitted^{-1}$

This leads to a flux over this kernel of $\Phi_{C1K\,HE} = T_{54} * NF$

$\Phi_{C1K\,HE} = 5.19 * 10^5 n * cm^{-2} * s^{-1}$

Tally 64 and its multiplier measures the fission rate per volume per emitted neutron over the kernel of one particle. Here, the tally applies to the inner part of the kernel, thus the tallied material is UO_2.

1tally 64 nps = 15000000
tally type 4 track length estimate of particle flux.
tally for neutrons

volumes

cell: 1

6.58433E-05

cell (1<7[0 0 0])

multiplier bin: -1.00000E+00 1 -6

2.39828E-02 0.0537

$T_{64} = 2.39828 * 10^{-2} \text{ fission} * cm^{-3} * neutron\_emitted^{-1}$

Cell volume is $V_C = 6.58433 * 10^{-5} cm^3$

This leads to a fission rate over cell1 (which is only the UO_2 part of the "central kernel") of

$FR_{C1K\,HE} = T_{64} * V_C * NF$

$FR_{C1K\,HE} = 4.00 * 10^{1}\ fission * s^{-1}$

We are interested in the total fission rate in the pebble. Therefore, tallies 54 and 64 applied to one cell/kernel in the lattice. Then volume normalization in tally 64 was done for only one particle to get particle results, or by 9560 particles for pebble results.

8.3.3 Randomly generated pebble

Tally 4 measures the neutron flux over cell 10 per emitted neutron. Here the tally namely applies to the inner part of the kernel (UO_2) that will be duplicated in the random particle structure. Therefore, it actually represents an integral over all kernels.

1tally 4 nps = 10000000

tally type 4 track length estimate of particle flux. units 1/cm**2

tally for neutrons

volumes

cell: 10

6.62384E-05

cell 10

2.35793E+02 0.0018

$T_4 = 2.35793 * 10^2 \,\mathrm{n} * cm^{-2} * neutron\_emitted^{-1}$

This leads to a flux over all kernels of $\Phi_{C9560KR} = T_4 * NF$

$\Phi_{C9560KR} = 5.99 * 10^9 n * cm^{-2} * s^{-1}$

For one particle, this result should be divided by the total amount of particles: 9560

$\Phi_{C1KAR} = T_4 * NF / 9560$

$\Phi_{C1KAR} = 6.26 * 10^5 n * cm^{-2} * s^{-1}$

Tally 14 and its multiplier measure the fission rate over cell 10 per volume per emitted neutron. Here the tally applies to the inner part of the kernel, thus the tallied material is UO_2. Again, as cell 1 will be duplicated in the random structure, it actually represents an integral over all kernels.

1tally 14 nps = 10000000
tally type 4 track length estimate of particle flux.
tally for neutrons

volumes
cell: 10
6.62384E-05

cell 10
multiplier bin: -1.00000E+00 1 -6
3.01449E+02 0.0017

$T_{14} = 3.01449 * 10^2 \,\mathrm{fission} * cm^{-3} * neutron\_emitted^{-1}$

Cell 1 volume is $V_{C1} = 6.58433 * 10^{-5} cm^3$

This leads to a total/integral fission rate in the pebble of $FR_{C9560KR} = T_{14} * V_{C1} * NF$

$FR_{C9560KR} = 5.03 * 10^5 \, fission * s^{-1}$

We are interested in the total fission rate in the pebble. Therefore, Tallies 4 and 14 apply to the cell that is duplicated into the random lattice. Indeed, this cell collects the flux of each particle. Then volume normalization was done for one particle only.

Tally 24 measures the neutron flux per emitted neutron over the kernel of one particle, precisely the one lying in the center of the pebble.

1tally 24 nps = 10000000
tally type 4 track length estimate of particle flux. units 1/cm**2
tally for neutrons

volumes
cell: 10
6.62384E-05

cell (10<16)
2.55955E-02 0.0444

$T_{24} = 2.55955 * 10^{-2} \mathrm{n} * cm^{-2} * neutron\_emitted^{-1}$

This leads to a flux over this kernel of $\Phi_{C1KR} = T_{24} * NF$

$\Phi_{C1KR} = 6.50 * 10^{5} n * cm^{-2} * s^{-1}$

Tally 34 and its multiplier measure the fission rate per volume per emitted neutron over the kernel of one particle in the center of the pebble. Here, the tally applies to the inner part of the kernel, thus the material is UO_2.

1tally 34 nps = 10000000
tally type 4 track length estimate of particle flux.
tally for neutrons

volumes
cell: 10
6.62384E-05

cell (10<16)

multiplier bin: -1.00000E+00 1 -6
2.49482E-02 0.0686

$T_{34} = 2.49482 * 10^{-2} \text{fission} * cm^{-3} * neutron\_emitted^{-1}$

Cell volume is $V_C = 6.58433 * 10^{-5} cm^3$

This leads to a fission rate in the center particle of the pebble of $FR_{C1K\,E} = T_{64} * V_C * NF$

$FR_{C1K\,R} = 4.17 * 10^{1}\, fission * s^{-1}$

We are interested in the total fission rate in the pebble. Therefore, tallies 24 and 34 applied to one cell into the random lattice. Then volume normalization was done for only one particle to get particle results or by 9560 particles for pebble results.

8.4 Summary of results and interpretation

8.4.1 Neutron flux

Simulation	Neutron flux	Unit
Φ C1 HO	5.3e+5	neutron/s/cm^2
Φ C8 HE	5.28e+5	neutron/s/cm^2
Φ C9560K HE	4.82e+9	neutron/s/cm^2
Φ C1KA HE	4.04e+5	neutron/s/cm^2
Φ C1K HE	5.19e+5	neutron/s/cm^2
Φ C9560K R	5.99e+9	neutron/s/cm^2
Φ C1KA R	6.26e+5	neutron/s/cm^2
Φ C1K R	6.5e+5	neutron/s/cm^2

Considering the flux results given in the above table, we conclude the following:

- The flux calculated by the two different methods (homogeneous mixture of the particle fuel and graphite and the heterogeneous distribution of particles in the regular square lattice) is quite similar. This means that, in this case, the geometry is not significantly interfering with cell averaged flux calculation.
- However, comparison between the regular lattice and random structure approaches shows a considerable difference in the flux calculated in the pebble. This can be partially explained by a shielding effect from particles. Further investigation is needed to confirm this hypothesis.

8.4.2 Fission rates

Simulation	Fission rate	Unit
FR HO	4.44E+05	fission/s
FR C8 HE T14	4.38E+05	fission/s
FR C8 HE T24	4.43E+05	fission/s
FR C9560K HE	3.87E+05	fission/s
FR C1K HE	4.00E+01	fission/s
⇒ FR C1K HE * 9560	3.83E+05	fission/s
FR C9650K R	5.03E+05	fission/s
FR C1K R	4.17E+01	fission/s
⇒ FR C1K R * 9558	3.98E+05	fission/s

The above table shows different ways how the fission rate in the pebble was calculated. The following conclusions can be made:

- Tallies 14 and tally 24 apply to the homogeneous tallying procedure in the regular lattice structure model. Tally 14 of the lattice case is slightly lower than the others due to an approximate atomic density specified in the tally.
- The tallying of the fission rates in the particle of the regular lattice geometry yields a slightly lower fission rate. There can be two reasons for this:
  - A geometry shielding effect of particles closer to the source on the others,
  - A larger amount of neutrons that pass through the pebble without interfering with particles/fuel ("neutron streaming").
- The above mentioned effects are less pronounced in the random structure compared to the regular lattice model as particles are placed in a stochastic way. This, also in comparison with the homogeneous structure modeling, leads to a higher fission rates.
- This is also stressed by the comparison of the central particle fission rate and the averaged one.

In terms of geometry, the random structure is more accurate to the reality than the two others. Therefore, its results seem to be more relevant. In all cases, the resulting fission rate in the pebble is estimated being between 3.87E+5 and 5.03E+5 fissions per second.