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Document title

DETERMINISTIC FP RELEASE STUDY

Executive summary

In this document, we describe models of diffusion and calculations performed with the ATLAS code, based on the conditions of HFR-P4 and HFR-EU1 experiments. We also study sensibility to the parameters, and to the failure of some layers.
1D, 2D and 3D calculations are presented.
The sensibility to the parameters is substantially high and the uncertainties on these parameters make results at present rough.

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Service d'études et de simulation du comportement des combustibles

CADARACHE

HTR particle deterministic fission product release study.

Etude déterministe du relâchement des produits de fission des particules RHT.

MICHEL Frédéric

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HTR PARTICLE DETERMINISTIC FISSION PRODUCT RELEASE STUDY. ETUDE DÉTERMINISTE DU RELÂCHEMENT DES PRODUITS DE FISSION DES PARTICULES RHT.

Auteur(s)	**MICHEL Frédéric**

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Résumé :

In this document, we describe models of diffusion and calculations performed with the ATLAS code, based on the conditions of HFR-P4 and HFR-EU1 experiments. We also study sensibility to the parameters, and to the failure of some layers.
1D, 2D and 3D calculations are presented.
The sensibility to the parameters is substantially high and the uncertainties on these parameters make results at present rough.
This document constitute the deliverable D-FT4.2 of RAPHAEL project, SP Fuel Technology.

Nous décrivons dans ce document une modélisation de la diffusion et des calculs réalisés avec le code ATLAS, basés sur les conditions des irradiations expérimentales HFR-P4 et HFR-EU1. Nous étudions aussi la sensibilité aux paramètres des modèles et à la rupture de certaines couches.
Des résultats de calculs 1D, 2D et 3D sont présentés.
La sensibilité aux paramètres est élevée et les incertitudes sur ces paramètres font que les résultats d'ATLAS sont pour l'instant peu précis.
Ce document constitue le livrable D-FT4.2 du projet RAPHAEL, SP Fuel Technology.

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LISTE DE DIFFUSION

DIFFUSION EXTERNE

SOCIÉTÉ	NOM DU DESTINATAIRE	NOMBRE D'EXEMPLAIRES	OBSERVATIONS
AREVA-NP/PARIS	D. HITTNER	®	® : RÉSUMÉ
AREVA-NP/LYON	M. PASQUET P. MAILHE P. GUILLERMIER	® 1 1	
EDF/R&D/MMC	S. LECLERCQ	1	

DIFFUSION INTERNE

Dpt/Service/Labo	NOM DU DESTINATAIRE	NOMBRE D'EXEMPLAIRES	OBSERVATIONS
DEN/DDIN/CCC	P. BROSSARD	®	
DEN/DDIN/DPSF	P. ANZIEU	®	Document disponible sur INTRADEC
DEN/DM2S/SERMA/LCA	X. RAEPSAET	1	® : RÉSUMÉ
DEN/DTN/SMTM		1	
DEN/DER/SESI	D. BARBIER	®	
DEN/DER/SESI/HTREX		PDF	
DEN/DEC	G. FLAMENBAUM	®	
DEN/DEC/SPUA/LMPC		1	
DEN/DEC/SPUA/LCU		1	
DEN/DEC/SESC		1+®	
DEN/DEC/SESC/LC2I		®	
DEN/DEC/SESC/LIPA	M. PHELIP	1	
	T. LAMBERT	®	
DEN/DEC/SESC/LLCC		®	
DEN/DEC/SESC/LSC		1	
	D. PLANCQ (PLÉIADES)	1	
	F. MICHEL	1	
	M. PELLETIER	1	
	TOUS SALARIÉS	® PAR @	

RÉVISIONS

DATE	OBJET DES RÉVISIONS	INDICE
OCTOBRE 2006	ÉMISSION INITIALE	0

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0. INTRODUCTION

The diffusion of fission product is an important phenomena of HTR reactors particle behavior. First, a low release of fission product is the main requirement of the particle. Secondly, the release rate is the only in-pile measurement that gives information on all particles' behavior.

This document describes the simulation of the diffusion of chemical elements and gives some simulation results performed with ATLAS code.

ATLAS is a software dedicated to the simulation of HTR particle behavior which includes the simulation of fission products diffusion. Its development is made at CEA in the simulation code framework PLEIADES. It uses the models gathered by the simulation working group of HTR-F program of European Community ; the models are mainly described in [2]. This work is extended in the RAPHAEL project, SP Fuel Technology.

Thermo-mechanical results of ATLAS are described in [1].

1.0. FINITE ELEMENT MODELING OF DIFFUSION

The diffusion of the fission products is solved by analogy with heat conduction. The problem is expressed in terms of activity diffusion. The analogy is made between the temperature and the activity. The activity is equivalent to the concentration for a metallic fission product, and it is equivalent to the partial pressure for a gaseous fission product. Corresponding equation is :

$$C_A \frac{\partial A}{\partial t} = div\left(D_A . \vec{\nabla} A\right) + q$$

Where : A is the activity (dimensionless by convention)

D_A the activity diffusion coefficient ($mol.m^{-1}.s^{-1}$)

q is the source term = fuel FP creation + negative proportional term corresponding to disintegration ($mol.m^{-3}.s^{-1}$).

C_A is the concentration over activity ratio ($mol.m^{-3}$)

In most cases, we will take C_A=1 and D_A=D, the diffusion coefficient, and the equation becomes the diffusion equation specified in [2].

This diffusion equation is solved on the mesh of the particle or of the fuel element with a finite element scheme. The Finite Element model is isotropic. The resolution is transient and linear.

At the end of a diffusion step, the cumulated released fraction (*F*) and the instantaneous release rate over birth rate ratio (*R/B*) of the studied isotopes are calculated.

The resolution of diffusion uses temperature to actualize diffusion coefficients. It also uses the displacement fields at current and previous times (results of the mechanical analysis) to preserve the quantities when the deformation state of the geometry is updated. Besides, the evolution of the thicknesses of the gas joints can have an effect on their resistance to diffusion, when the gas is not supposed to be transparent.

The advantage of using activity in place of concentration is that we can have different concentrations at equilibrium in the different materials.
It is for example the case for gases which mainly stay in gap (fig below), but it should be the case for all isotopes in every material. For gases, we consider a retention capability proportional to open porosities.

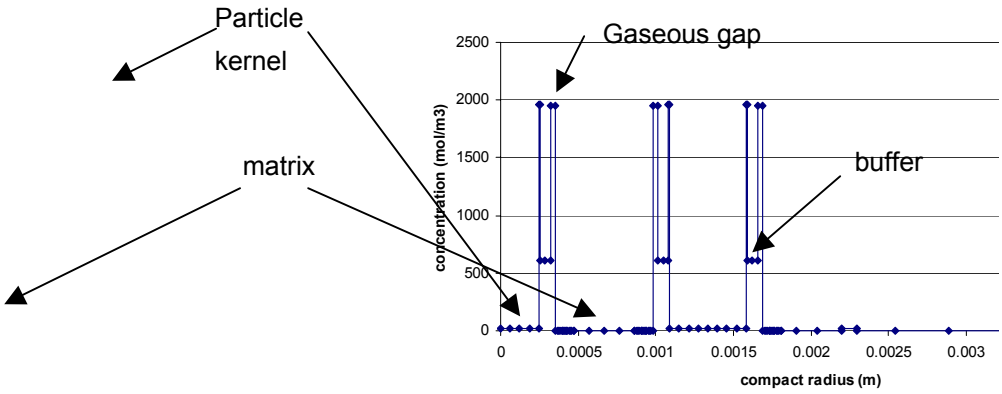

FIGURE 1 : ACTIVITY (LEFT) AND CONCENTRATION (RIGHT) PROFILES OF ONE GAS THROUGH ONE HALF AND ONE PARTICLE IN A FRAGMENT OF FUEL ELEMENT IN A QUASI STEADY STATE.

An other example of difference between concentration and activity can take place at the surface of the graphite near the coolant for some elements where there is an interface over-concentration :

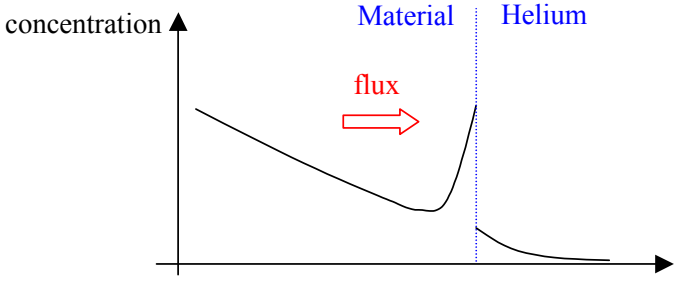

FIGURE 2 : SCHEMA OF CONCENTRATION PROFILE WHEN INTERFACE HOLD A GREAT QUANTITY OF THE ELEMENT.

This last possibility is not yet used in Atlas.

1.1. TRANSFER MODELLING AT COOLANT INTERFACE

The transfer of the fission products into the coolant is simulated when the geometry is the HTR compact fuel element. The analogy with thermal analysis is kept for transfer : the outgoing flux on the interface between the structural bloc and the coolant is determined by the product of a transfer coefficient by the concentration step between the two media.
In this case, the Finite Element model is completed with a pseudo-convection model defined for the outer face of the structural bloc.

- The concentration step between the two media is determined by an empirical correlation describing the **sorption/evaporation** phenomena. The concentration of the considered fission product in Helium is supposed to be proportional to the one on the adjacent solid phase (structural graphite bloc) :

$$C_{FP}^{He} = \alpha \times C_{FP}^{solid}$$

α is the evaporation coefficient. It is described by an empirical function of the temperature at the solid/gas interface :

$\alpha = 0$	for $T < 773$ K
$\alpha = -3{,}4785 + 4{,}5.10^{-3} \times T$	for $773 \leq T \leq 973$ K
$\alpha = 0{,}9$	for $T > 973$ K

- The transfer coefficient is evaluated according to an empirical law extracted from [6], pp 484-488. The formula used by ATLAS V2.1 corresponds to forced convection with a turbulent flow in a tube (Reynolds number ≥ 2100). The transfer coefficient is given by

$$h = \frac{D}{d} \times 0{,}023 \times Re^{0{,}8} \times Sc^{0{,}33} \qquad \text{(m/s)}$$

with D (m^2/s) Diffusion coefficient of the fission product in Helium
d (m) Hydraulic diameter = Diameter of the Helium channel
Re (-) Reynolds number $Re = \frac{\rho V d}{\mu} = \frac{V d}{\nu}$

with ρ (kg/m^3) Density of Helium
μ (kg/(m.s)) Dynamic viscosity of Helium
ν (m^2/s) Kinematic viscosity of Helium
V (m/s) Average coolant velocity

Sc (-) Schmidt number $Sc = \frac{\mu}{\rho D} = \frac{\nu}{D}$

- The outgoing flux on the interface between the structural bloc and the coolant is finally established :

$$\varphi = h \times (1-\alpha) \times C_{FP}^{solid} \qquad \text{(mol/m}^2\text{/s)}$$

with	α	(-)	Evaporation coefficient, as previously defined
	h	(m/s)	Transfer coefficient, as previously defined
	C_{FP}^{solid}	(mol/m^3)	Concentration of the considered fission product on the outer face of the structural bloc

1.2. BOUNDARY CONDITIONS

The default modeling of diffusion uses the implicit boundary condition for Finite Element models : null flux on the frontiers of the domain. This adiabatic condition insures the conservation of the quantities over the full domain ; this allows to evaluate the release from the particles (released fraction and release rate over birth rate R/B), when the model includes at least one additional material medium surrounding the particles. However, it is possible to impose a null activity on the outer bound of the domain.
As an alternative, the model used for the HTR compact fuel element allows to simulate the transfer of the fission products into the coolant, by imposing a pseudo-convective boundary condition on the interface between the structural bloc and the coolant. This has been described in the previous chapter.

1.3. SOURCE TERM FOR DIFFUSION

The load for diffusion is defined by source terms, corresponding to the creation of elements into the kernel of the particles, by the fission reactions. The source terms depends on the fission density, multiplied by the fission yield which is specific for each species. The fission yield is usually an empirical function of burn-up, and depends on the irradiation conditions and on the composition of the fuel (especially uranium enrichment).
The product of fission density by fission yield determines the intragranular source term. For a metallic species, the intragranular source term is the load for diffusion. For a gaseous species, this term has to be multiplied by the release rate from grains, in order to obtain the fraction of the source passing into the open porosities and available for macroscopic diffusion.

2. "RELEASED FRACTION" AND "RELEASE RATE TO BIRTH RATE" CALCULATIONS

2.0. CALCULATIONS RELATIVE TO THE HTR PARTICLE

The released fraction is calculated as the ratio of the quantities escaped out of the particle over the quantities born into the kernel. The layers to be considered as out of the particle are previously defined.

The released fraction (*F*) is calculated by the general formula given below :

$$F = \frac{Q_{out}}{Q_{Init} + Q_{Prod}}$$

where Q_{out} is the quantity of the fission product outside the particle, obtained by integrating the concentration field in the corresponding layers.

Q_{Init} is the quantity at initial time ; this quantity has to be taken into account for an initial filling gas which can also be a fission product (Xenon for example).

Q_{Prod} is the quantity produced into the fuel kernel since initial time ; it is updated by integrating the birth rate during the time step

$$Q_{Prod} := Q_{Prod} + \frac{\partial Q_{Prod}}{\partial t} \times dt$$

$\frac{\partial Q_{Prod}}{\partial t}$ is obtained by integrating the volumetric source field in the kernel.

The release rate to birth rate ratio (*R/B*) is calculated by the general formula given below :

$$R/B = \frac{\frac{\partial Q_{out}}{\partial t}}{\frac{\partial Q_{Prod}}{\partial t}} \quad \text{where} \quad \frac{\partial Q_{out}}{\partial t} = \frac{Q_{out}(t) - Q_{out}(t - dt)}{dt}$$

$\frac{\partial Q_{Prod}}{\partial t}$ as previously defined

2.1. CALCULATIONS RELATIVE TO THE HTR FUEL COMPACT ELEMENT

When the geometry is the HTR compact fuel element, the transfer of the fission products into the coolant is simulated. The outgoing flux on the interface between the structural bloc and the coolant is determined by the product of a transfer coefficient by the concentration step between the two media.

In this case, the release rate from the compact is calculated by integrating the outgoing flux on the transfer surface :

$$\frac{\partial Q_{out}}{\partial t} = \iint_{S_{trans}} h \, \Delta c \, dS$$

The birth rate $\frac{\partial Q_{Prod}}{\partial t}$ is still obtained by integrating the volumetric source field in the fuel kernels.

Using these quantities, the release rate to birth rate ratio (*R/B*) is determined by the same formula as this already seen in the previous chapter :

$$R/B = \frac{\frac{\partial Q_{out}}{\partial t}}{\frac{\partial Q_{Prod}}{\partial t}}$$

The released fraction from the compact (*F*) is also calculated by the general formula :

$$F = \frac{Q_{out}}{Q_{Init} + Q_{Prod}}$$

where Q_{out} is the quantity of fission product released into the coolant ; it is updated by integrating the release rate during the time step

$$Q_{out} = Q_{out} + \frac{\partial Q_{out}}{\partial t} \times dt$$

Q_{Init} and Q_{Prod} as defined in the previous chapter.

3. GAS BEHAVIOUR

3.0. FUEL KERNEL RELEASE RATE

There is a specific model for gas release from intra granular location to open porosities of kernel. This kernel release rate model takes into account diffusion trough UO_2 so the diffusion coefficient further used in finite elements resolution must be imposed as high trough UO_2 grains.
Fuel release rate in Atlas is a function of FIMA and temperature, as presented below :

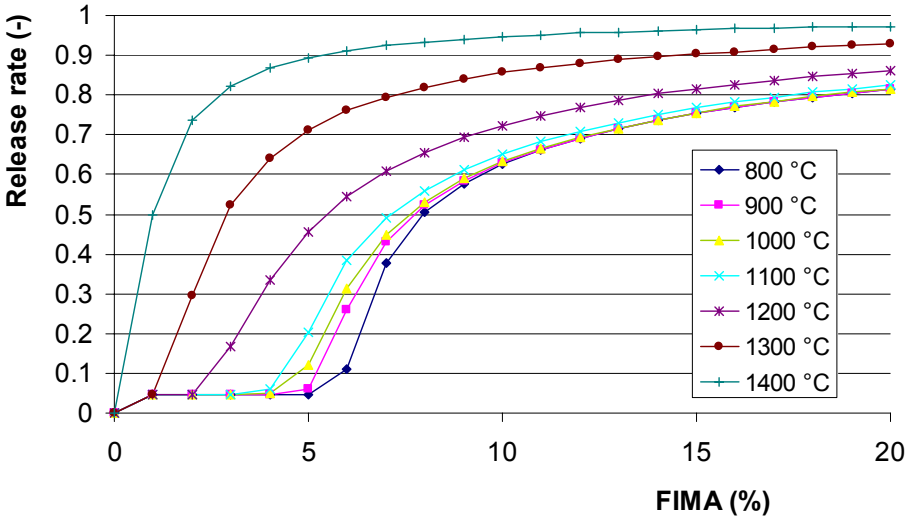

FIGURE 3 : UO_2 KERNEL RELEASE RATE

For gases, this model already takes into account diffusion through kernel. For metallic products, this model is not used and fuel grain release rate has the value of 1. For metallic FP, we keep material diffusivity at macroscopic scale. For impermeable layers, the macroscopic diffusivity equals microscopic diffusivity.

3.1. STATE LAW FOR GAS

The state of the gas mixture is described in first approximation by the perfect gas law. The expansion volume in each material is determined by the open porosity ratio. For each gaseous species in the mixture, the perfect gas law is established :

$$P_i \xi V = n_i RT \Rightarrow C_i = \frac{n_i}{V} = \frac{P_i \xi}{RT}$$

where P_i (Pa) is the partial pressure of the considered species

ξ (-) is the open porosity ratio and ξV (m^3) the expansion volume

n_i (mol) is the quantity of the considered species

R is the perfect gas constant, R=8.314 J/mol/K

T (K) is the temperature

3.2. OXYGEN GENERATED PER FISSION

For the number of oxygen per fission (opf), we use the proksch formula from [2].

$$\log_{10}\left(\frac{opf}{t^2}\right) = -0.21 + \frac{-8500}{T}$$

t is the time (in days)

T is the temperature (K)

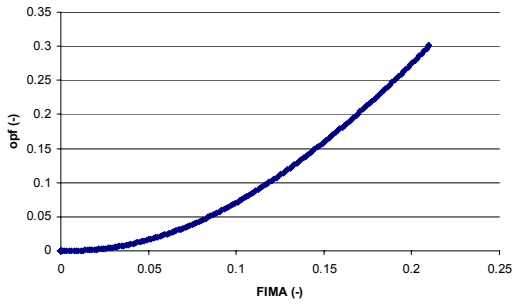

FIGURE 4 : EXAMPLE OF OPF EVOLUTION

3.3. CO/CO_2 EQUILIBRIUM

The oxygen partial pressure is first calculated as the weighted sum of CO and CO_2 partial pressures, obtained at the preceding time step :

$$P_O = P_{CO} + 2.P_{CO_2} \qquad \text{(Pa)}$$

The new CO and CO_2 local partial pressures are then determined according to the oxygen partial pressure and the local temperature T (K) at current time, by the following expressions :

$$Kp = \exp\left(18.36 - \frac{19970}{T}\right).10^6 \qquad \text{(Pa)}$$

$$f = \frac{\sqrt{Kp^2 + 8.Kp.P_O} - Kp}{4.P_O} \qquad \text{(-)}$$

$$P_{CO} = f.P_O \qquad \text{(Pa)}$$

$$P_{CO_2} = \frac{1-f}{2}.P_O \qquad \text{(Pa)}$$

This model determines differential pressures in the gas joints when the temperature itself is heterogeneous. This instability induces the amoeba effect, but there is actually in ATLAS no available correlation between the kernel migration model and the CO/CO_2 equilibrium model.

4. DIFFUSION COEFFICIENTS

ATLAS includes already some coefficients from AIEA TECDOC or other sources.

	Cs	Xe	CO	Kr	I	Ag	Sr	Pd	Nd
UO2	A + F	A			A	A	A		
Dense PyC	A + F	A				A	A		
SiC	A + F	A				A	A		
Compact	A + F				A	A	A		
Graphite	A + F				A	A	A		

A : from AIEA TECDOC [3].

F : from Framatome contribution of [2].

TABLE 1 : DIFFUSION COEFFICIENTS INCLUDED IN ATLAS

Ag110m, Cs137 and Sr90are the only isotopes for which all the data needed for the calculation are available. There are many lacks, for example to calculate **Kr** R/B to be compared to on line measurement of HFR-P4 experiment [4].

The diffusion coefficients are most often a function of temperature. For Ag, Cs and Sr, we can plot them for each material :

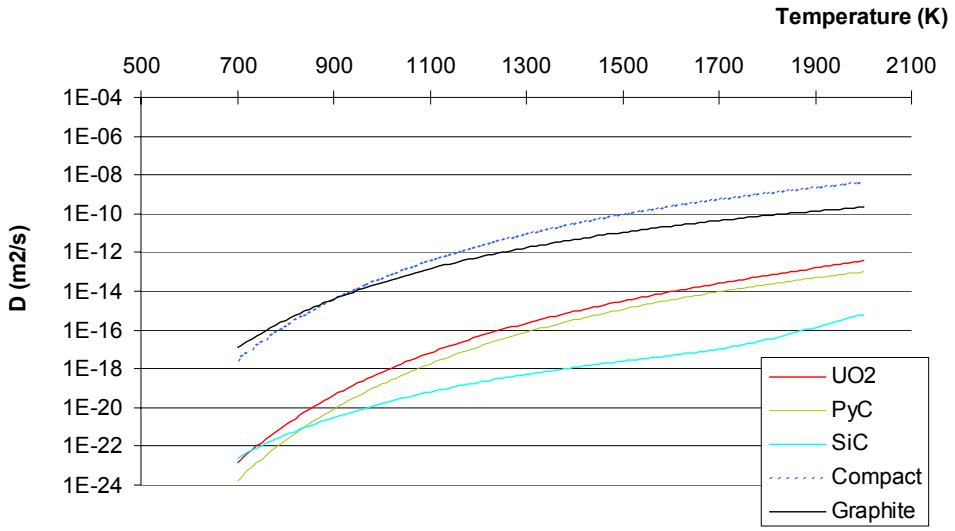

FIGURE 5 : DIFFUSION COEFFICIENTS FOR CS

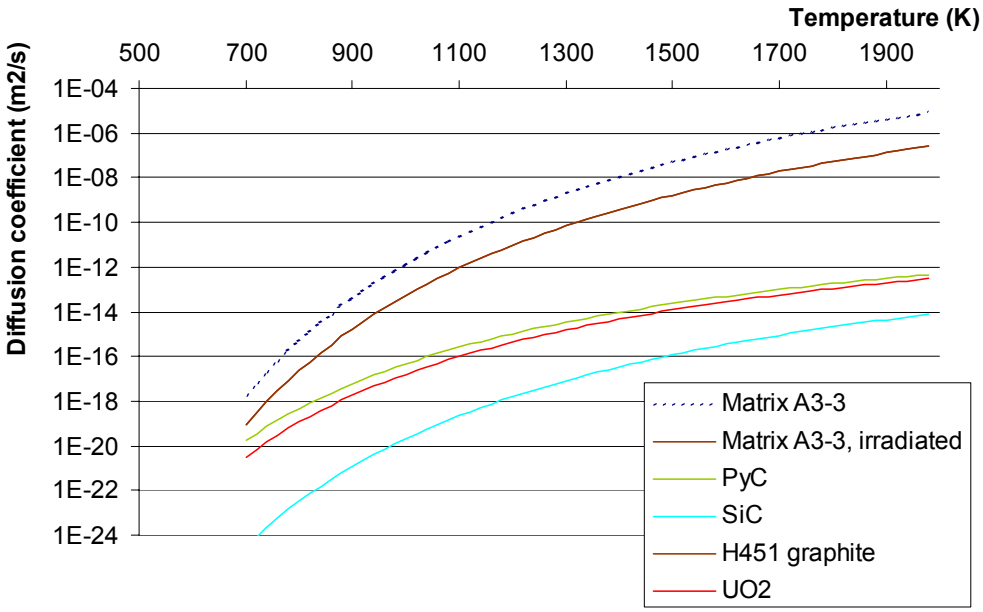

FIGURE 6 : DIFFUSION COEFFICIENTS FOR AG

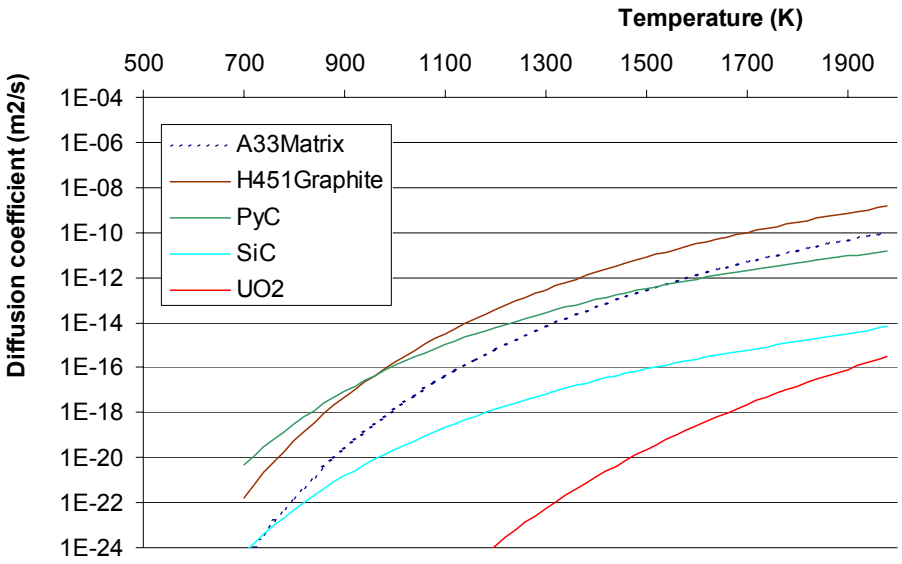

FIGURE 7 : DIFFUSION COEFFICIENTS FOR SR

With these values and standard TRISO layer thicknesses, we can evaluate 2 diffusion characteristic times :

- The characteristic time for diffusion to reach the other side of one wall : $t_{c1} = \left(\sum \frac{th}{\sqrt{D}} \right)^2$
- The time for all the content of a spherical thin shell to pass through the shell : $t_{c2} = \frac{d}{6} \sum \frac{th}{D_A} = \frac{d}{6} \sum \frac{aoc.th}{D}$

th : layer thickness (m)

With activity==concentration, and for Ag at 1300K we have the following values :

	Thickness	D	Th/D	$Th/D^{0.5}$
PyC	4.00E-05	3.4376E-15	1.16E+10	6.82E+02
SiC	3.50E-05	8.2639E-18	4.24E+12	1.22E+04

TABLE 2 : DIFFUSION CHARACTERISTICS OF PYC AND SIC LAYERS

With d= 500 µm, we have :

	t_{c1}	t_{c2}
SiC alone	$1.48\ 10^8$	$3.53\ 10^8$
SiC + PyC	$1.83\ 10^8$	$3.55\ 10^8$

TABLE 3 : DIFFUSION CHARACTERISTIC TIMES OF PARTICLE LAYERS

In our assumption, we have considered thin shells. With the real particle geometry (thick shell in spherical geometry), the expression of characteristics times would be much more complicated. We will only say that it would sensibly increase t_{c1} and decrease t_{c2}.

In this case that is representative of some relatively high temperature situations, we can see that the irradiation time (600 days = 5.18 10^7s) is below but near this two characteristic times.

To have really low release, we must stay far below t_{c1}. For the time t_{c1}, although SiC layer is the main wall to diffusion, PyC layer is important. PyC failure will have sensible consequences on release rate.

An other consequence of those high orders is that release rate stay very low at the beginning of irradiation but will grow very quickly on logarithm scale and can be near 1 for high irradiation temperature or time.

5. EXAMPLE OF CALCULATION : HFR P4 EXPERIMENT

5.0. CONDITIONS

Conditions are taken from HFR P4/1 capsule irradiation :

Temperature of particles is near 1200 K, the Burn-Up is about 14% FIMA after 351 full power days.

Particle layer thicknesses are 94,41, 36 and 40μm for buffer, IPyC, SiC and OPyC respectively. Kernel diameter is 497μm.

After irradiation, an heating test at 1873K during 300 hours is realized.

5.1. ATLAS RESULTS

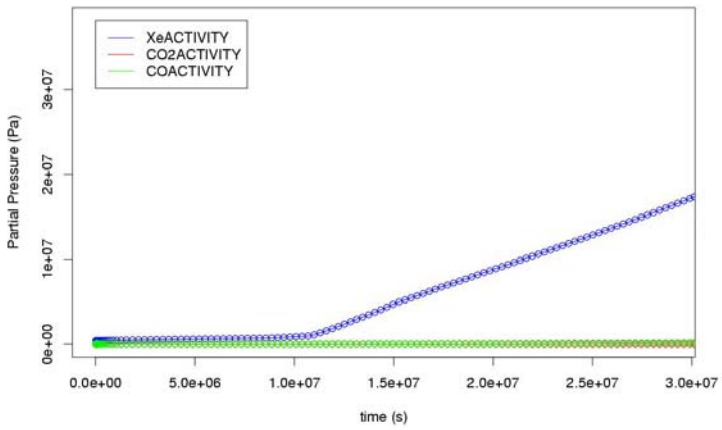

FIGURE 8 : EVOLUTION OF XE, CO AND CO_2 PARTIAL PRESSURES IN THE FREE VOLUME INSIDE THE PARTICLE AT 1200K.

Irradiation time and temperature being not so high, CO pressure stay far below pressure due to FP gases.

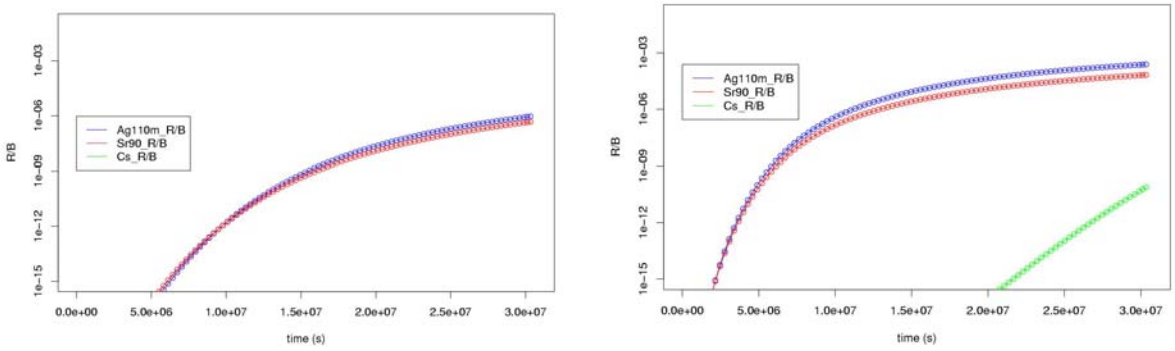

FIGURE 9 : R/B RESULTS DURING HFR-P4 IRRADIATION AT 1200 (LEFT) OR 1273 K (RIGHT)

We see here that a small difference of temperature can dramatically change release rate. With actual Cs diffusion coefficients, low in both SiC and PyC, Cs release is very low.

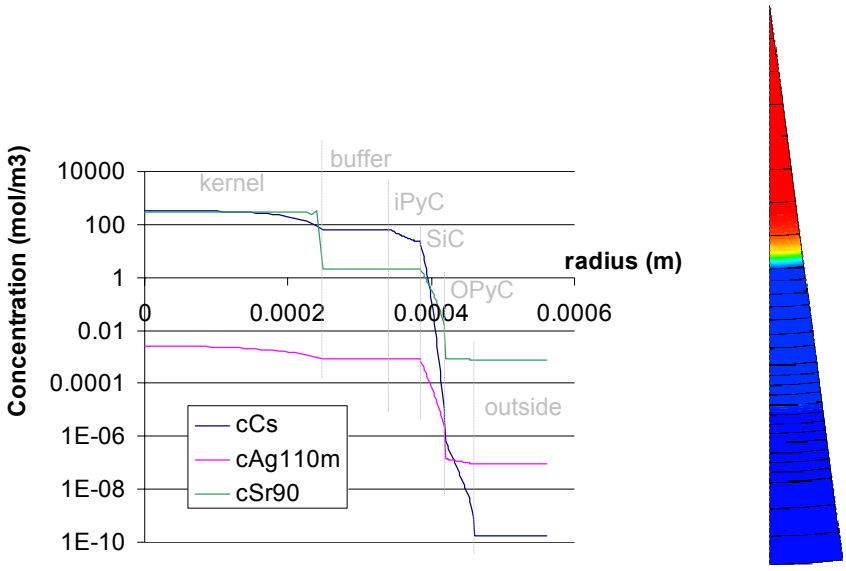

FIGURE 10 : CONCENTRATION PROFILE ALONG RADIUS AT END OF HFR-P4 IRRADIATION AT 1273 K.

We see in this graph that the kernel keeps the most part of its fission product. For Ag and Sr, PyC layers do not constitute a good protection against FP migration but SiC does.

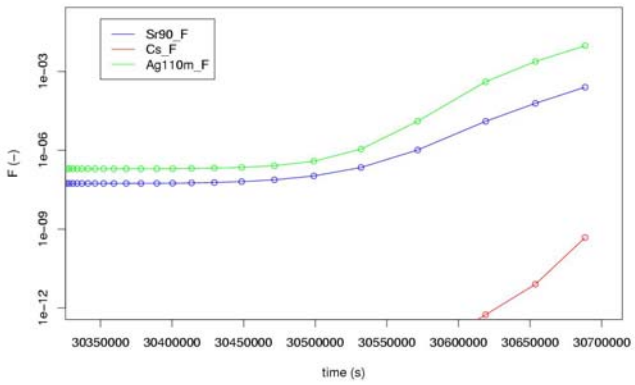

FIGURE 11 : RELEASE FRACTION DURING PI HEATING TEST.
IRRADIATION HFR-P4 AT 1200K, HEATING AT 1873 K

In this simulation, fractional release during heating test starts at the value of the end of irradiation and needs time to arrive at inflexion point. This behavior is due to the fact that we had no sensible diffusion between irradiation and heating, so the particle at the beginning of heating test is at the state of the end of irradiation. Cs release is very low.

Simulation results are higher for Sr and Ag than experimental results [4] but much lower for Cs fractional release. The results are not in agreement with HFRP4 results. To do validation, we will need to be closer to real experiments times and temperature variations, simulate the pebble matrix effect, take into account the statistic of particles and probably upgrade diffusion coefficients for Cs.

5.2. SENSIBILITY

We take as reference the calculation at 1273 K presented above. We have already seen great effect of temperature. We see below the effect of thickness variation and a variation of the parameter “activity over concentration” (aoc) (see §1.0).

	R/B at end of irradiation (-)
Reference calculation	2.42E-04
Double SiC aoc	1.27E-04
Half SiC aoc	4.43E-04
Half PyC aoc	1.14E-04
Sic thickness=33 μm	4.15E-04
PyC thicknesses=38-37 μm	2.52E-04

TABLE 4 : COMPARISON OF R/B VALUES, MODIFYING PARAMETERS

PyC aoc variation is about as influent as SiC aoc variation. This parameter has sensible effect and should be taken into account because its value could be some orders of magnitude different from 1.

FIGURE 12 : CONCENTRATION PROFILES FOR AG AT THE END OF IRRADIATION FOR DIFFERENT VALUES OF ACTIVITY OVER CONCENTRATION (AOC) VALUES

As sensibility is very high for all parameters, we can expect that the mean R/B for a group of particles will not be equal to the R/B value of the mean particle.

6. 2D SIMULATION WITH FAILED LAYERS

6.0. CONDITIONS

We take again conditions HFRP4 experiment at 1200K. In this simulation, the mesh includes :

- a flaw through IPyC layer
- the IPyC flaw and a partial debonding around the flaw between IPyC and SiC layer from –10° to 35° of horizontal axis (see image below).
- the previous flaw extended by a flaw through SiC layer, with a partial debonding between SiC and OPyC.

We will compare the diffusion through meshed failed layers with the diffusion trough 1D mesh with high diffusivity of IPyC layer.

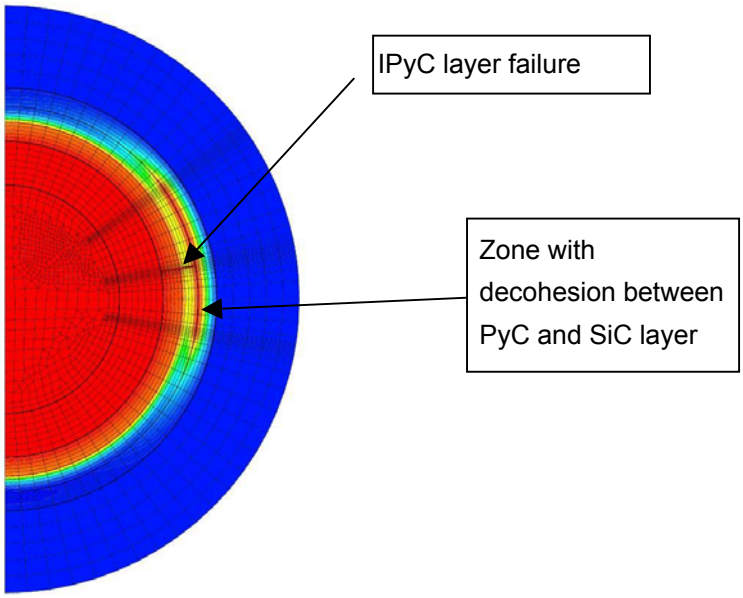

FIGURE 13 : CONCENTRATIONS IN FP FROM DIFFUSION THROUGH FLAW AND DEBONDING.

(TO DO THIS ILLUSTRATION WE IMPOSED A HIGH KERNEL DIFFUSIVITY).

6.1. ATLAS RESULTS

We present R/B values for the condition above :

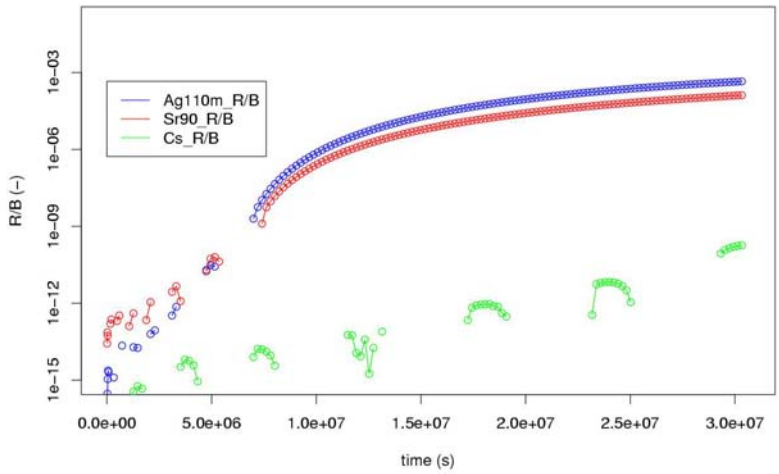

FIGURE 14 : HFR-P4 R/B CALCULATION, WITH IPYC CRACK AND PARTIAL DEBONDING

When release rate is too low, ATLAS fails to give an evaluation, but this is function of mesh refinement. When values are negative, the curve disappears on the logarithmic scale, hence the discontinuities. Cs R/B value is not correct here.

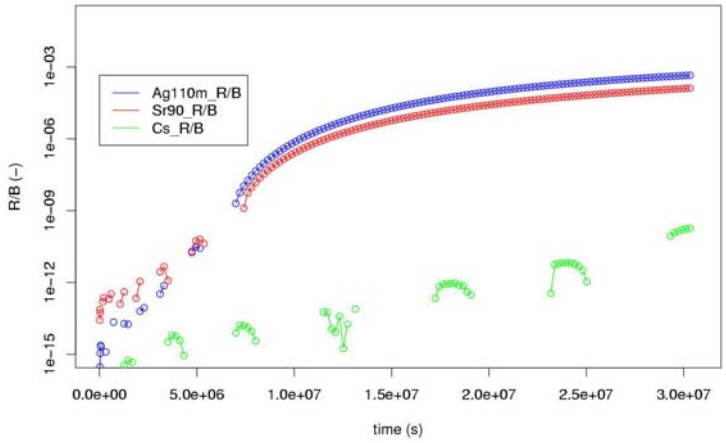

FIGURE 15 : HFRP4 IPYC CRACK WITH NO BEBONDING

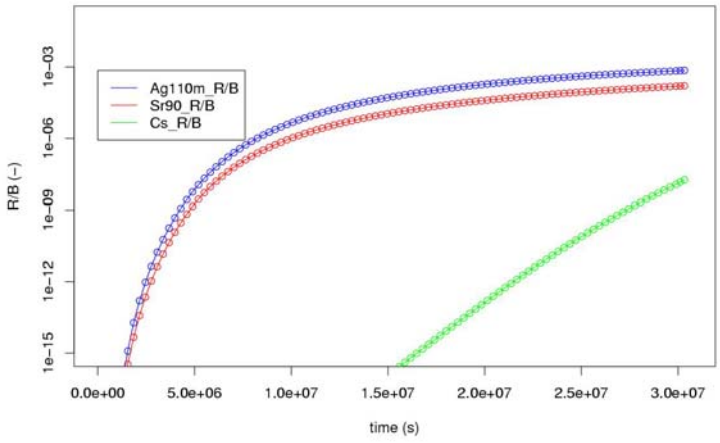

FIGURE 16 : R/B EVOLUTION OBTAINED WITH 1D MESH, WITH HIGH IPYC DIFFUSIVITY

If we put in a same table the results of previous calculations, we see that more the flaw is open, the more the release is high :

	R/B at end of irradiation (-)
Reference calculation	2.42E-04
IPyC failure	4.41E-04
IPyC failure and partial debonding	4.50E-04
High IPyC diffusivity	7.16E-04
High IPyC diffusivity and high IPyC aoc	10.12E-04

TABLE 5 : R/B VALUES FOR DIFFERENT PARTICLE FAILURES

If SiC fails, release rate becomes even higher.

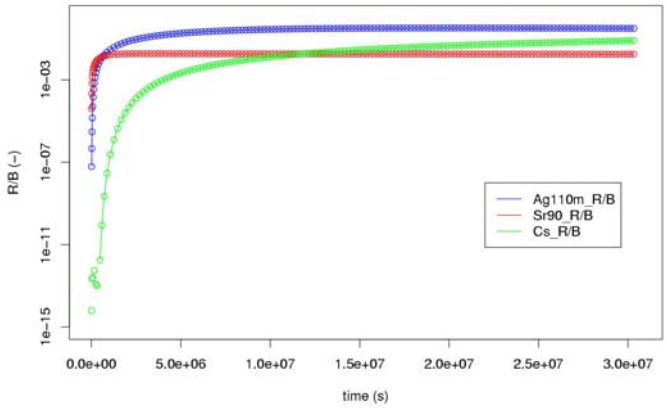

FIGURE 17 : IPYC AND SIC FAILURE WITH PARTIAL DEBONDING WITH OPYC

With OPyC only, the time to establish diffusion through layers becomes very low. Almost all metallic FP can go through OPyC. If R/B stays noticeably below 100% it is because the kernel keeps a good part of its FP. Cs is the last element to diffuse through particle layers.

7. ANOTHER EXAMPLE WITH HFR EU1 CONDITIONS

7.0. CONDITIONS

We perform a simulation with expected HFR-EU1 conditions, that is : end Burn-up of 22% FIMA reached in 600 efp days with an irradiation temperature of 1373 K.
Particles layer thicknesses are 94.9, 41, 35.4 and 40 μm for buffer IPyC SiC,and OPyC respectively. Kernel diameter is 502 μm.

7.1. ATLAS RESULTS :

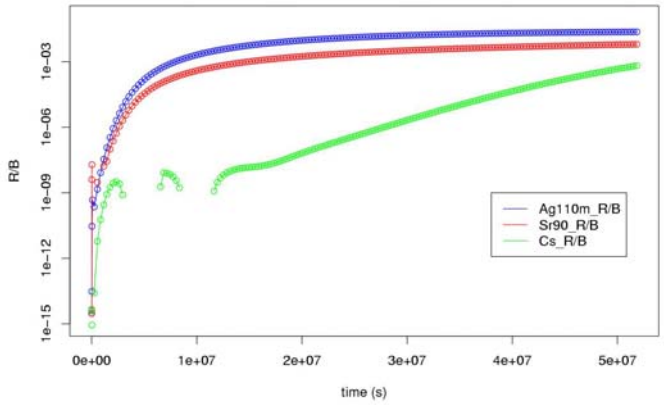

FIGURE 18 : R/B OF SR, AG AND CS OVER TIME DURING HFR-EU1 CALCULATION

As temperature is higher, release rate during irradiation should be much higher that what was obtained during HFR-P4 experiment.

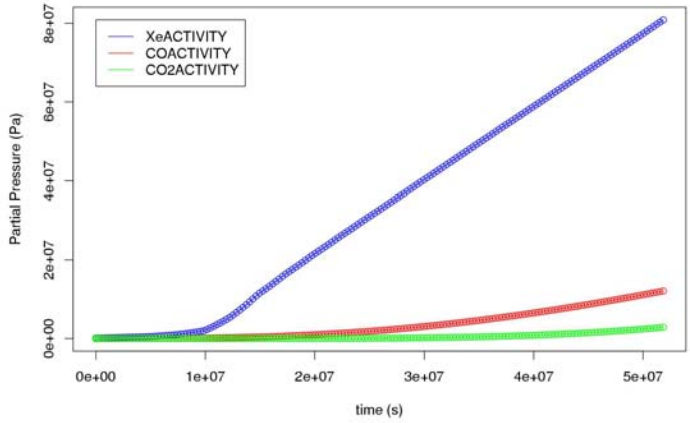

FIGURE 19 : CONTRIBUTION OF PRINCIPAL GASES TO INTERNAL PRESSURE DURING IRRADIATION

In this experiment, CO pressure stay below FP pressure but is not negligible.

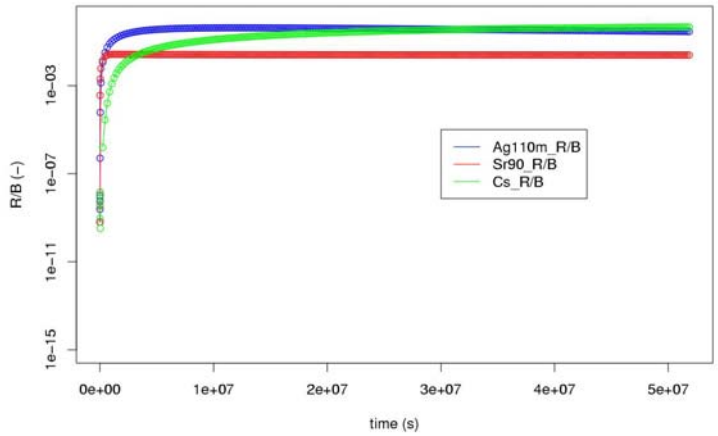

FIGURE 20 : HFR-EU1 ATLAS SOLUTION FOR R/B OVER TIME FOR AG, CS AND SR, WITH IPYC CRACK

Release rate is much higher that the previous results with intact particle. For Ag, we see that, due to self-disintegration and Kernel retention, only about 20% of Ag has the possibility to reach the external of the particle. After half time, the R/B value decrease for Ag110m because the disintegration also affect elements already outside and Atlas do not take correctly into account this effect.

8. THREE DIMENSIONAL SIMULATION OF FUEL ELEMENT AND GRAPHITE BLOCK

8.0. CONDITIONS

We simulate some particles in a cylindrical compact, roomed in a prismatic graphite block. This calculation is not representative of real GT-MHR geometry because of mesh element number limitation ; the mesh only include 3 particles in a radius of the fuel element. Real element should have about 5 particles in a radius. The conditions are the same as for HFR-P4 irradiation, except for geometry and temperature presented below.

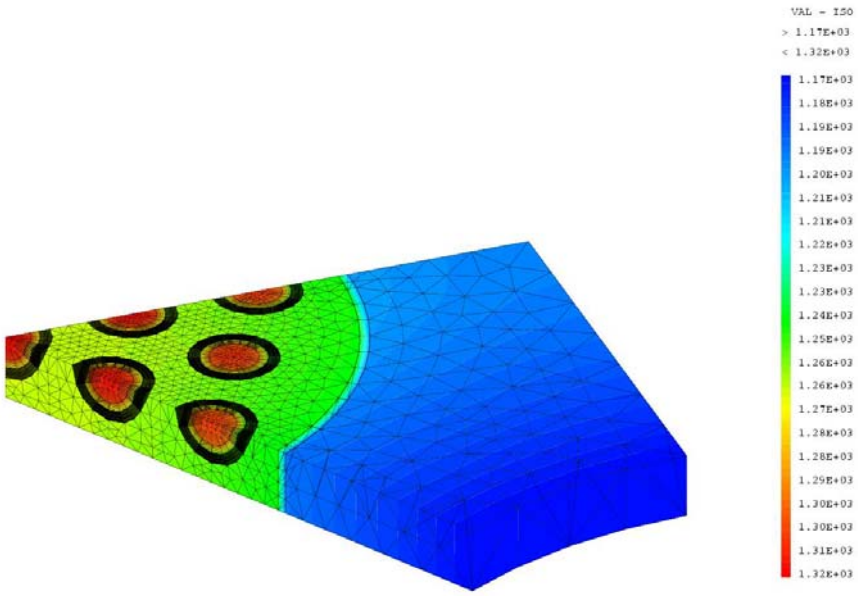

FIGURE 21 : TEMPERATURE FIELD DURING CALCULATION (K)

8.1. ATLAS RESULTS

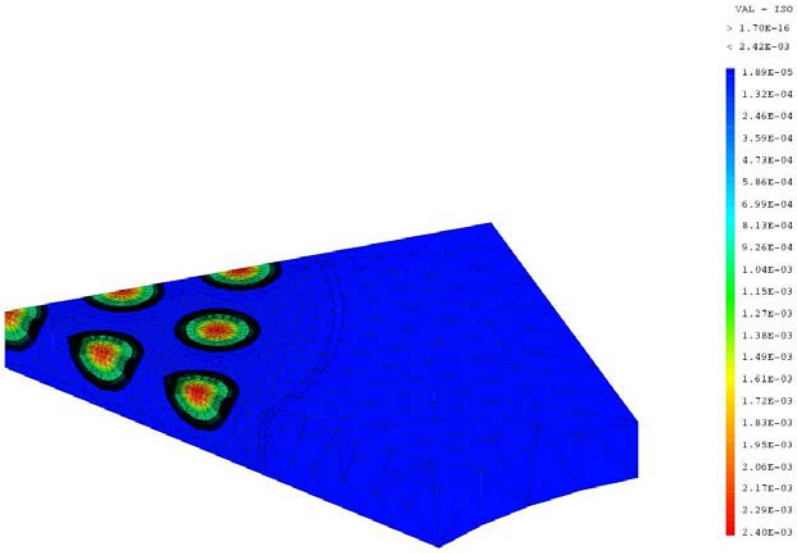

FIGURE 22 : AG ACTIVITY AT END OF IRRADIATION (-)

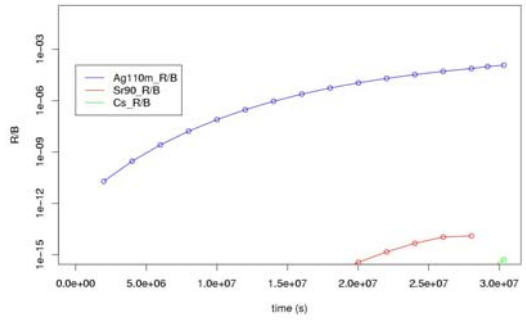

FIGURE 23 : R/B OF COMPACT DURING IRRADIATION (-)

In this case, the main difference between R/B of Ag and Sr is due to the important difference of diffusivity for these two elements in graphite. With a size of graphite more than 2 order of magnitude higher than layers, the first diffusion characteristic time through graphite for Sr is higher than those of SiC layer. Only Ag release rate is high (>1.E-6).

9. CONCLUSION

Fission products release from particle is very sensitive to conditions – particularly temperature - and to model coefficients. With all the uncertainties, we actually cannot expect an accurate evaluation of FP release rate with a code including these models, like ATLAS, but in the best case we could reach the order of magnitude of the release rate results. Before validation, simulation will require more precise models (perhaps taking into account interfacial segregation) and more accurate diffusion coefficients.
For this point, new irradiation tests are needed.

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