



EUROPEAN COMMISSION

5th EURATOM FRAMEWORK PROGRAMME 1998-2002

KEY ACTION : NUCLEAR FISSION



**HTR FUEL TECHNOLOGY STUDIES
COMPLEMENTARY ACTIVITIES TO HTR-F**

**CONTRACT N°
FIKI-CT-2001-00150**

Pre-calculation report on HFR-EU1 test

Frédéric MICHEL (CEA)

Dissemination level: CO
Document Number: HTR-F1-05/07-D-3.2.1
Final
Deliverable Number: 3.2



DIRECTION DE L'ÉNERGIE NUCLÉAIRE
DIRECTION DU CEA/CADARACHE
DÉPARTEMENT D'ÉTUDES DES COMBUSTIBLES
SERVICE D'ÉTUDES ET DE SIMULATION DU COMPORTEMENT DES COMBUSTIBLES

LABORATOIRE DE SIMULATION DES COMBUSTIBLES

**HTR-F1 PROJECT - DELIVERABLE N°3.2 : HFR-EU1 PARTICLE MEAN FAILURE PROBABILITY
EVALUATION WITH ATLAS V1.0.**

**PROJET HTR-F1 - DÉLIVRABLE N°3.2 : EVALUATION AVEC ATLAS V1.0 DU NOMBRE MOYEN DE
PARTICULES DÉFAILLANTES DE L'EXPÉRIENCE HFR-EU1.**

DE F. MICHEL

Note Technique SESC/LSC 05-022

Indice 0

de July 2005



Note Technique SESC/LSC 05-022

Indice 0

Page 1/28

Titre : HTR-F1 PROJECT - DELIVERABLE N°3.2 : HFR-EU1 PARTICLE MEAN FAILURE PROBABILITY EVALUATION WITH ATLAS V1.0.

PROJET HTR-F1 - DELIVERABLE N°3.2 : EVALUATION AVEC ATLAS V1.0 DU NOMBRE MOYEN DE PARTICULES DÉFAILLANTES DE L'EXPÉRIENCE HFR-EU1.

Auteur(s) : F. MICHEL

Résumé :

Cette note présente les résultats de simulation des particules de l'expérience HFR-EU1 avec l'application ATLAS V1.0 et un calcul statistique de la probabilité moyenne de rupture. Nous présentons des résultats obtenus avec 3 séries de propriétés de l'application d'ATLAS pour les couches de la particule simulée : « FZJ », « BNFL » et « CEGA ». Nous utilisons les lois « CEA » pour l'UO₂. Ces propriétés ont été produites par le groupe de travail européen HTR-F [1].

Le comportement de la particule est classique : le pyrocarbone (PyC) des couches densifie sous irradiation et comprime la particule et la couche de carbure de silicium (SiC). Cette augmentation de la contrainte est relaxée par le fluage du PyC sous irradiation et, à la fin d'irradiation, la pression interne contrebalance l'effet de la densification du PyC. Alors, la couche de SiC peut passer en traction et peut rompre.

Pour le calcul statistique du taux moyen de rupture, nous considérons une distribution gaussienne de l'épaisseur pour toutes les couches. Nous avons utilisé deux méthodes de calcul : un tirage d'importance (non optimisé) et une régression polynomiale des résultats. Le tirage d'importance permet d'atteindre une variance faible avec un échantillonnage plus faible, particulièrement pour des occurrences faibles.

Avec toutes les hypothèses prises ici, la première rupture due à l'irradiation de la couche SiC pourrait survenir avant la fin de l'expérience et devrait alors être suivie rapidement pour une quantité rapidement croissante de ruptures pour atteindre jusqu'à 0.1 % des particules.

Abstract :

This note presents the simulation results with the code ATLAS V1.0 and a statistical calculation of the mean particle failure probability of the particles of HFR-EU1 experiment.

We present results obtained with the 3 series of properties for the particle coating called "FZJ", "BNFL" and "CEGA" in the ATLAS application. We use "CEA" laws for UO₂. Those properties were produced by the HTR-F European working group [1].

The behaviour of the particle is classical : the pyrocarbon (PyC) layers shrink under irradiation and compress the particle and the silicon carbide (SiC) layer. This stress increase is relaxed by the PyC irradiation induced creep and, at the end of irradiation, the internal pressure counterbalances the PyC shrinkage effect. Then, the SiC layer can be in tension and can fail.

For the statistical calculation of the failure fraction, we consider a given gaussian thickness distribution for all coatings. We used two methods to perform the calculation : an importance sampling method (not optimised) and the use of a polynomial regression of the results of the code. The importance sampling permits to reach low statistical error with less numbering sample, especially for low occurrences.

With all hypothesis taken here, the first irradiation induced SiC failure could occurs before the end of the experiment and should then be followed by a rapidly increasing amount of particles to reach up to 0.1% of the particles.

Mots Clés

HFR-EU1, ATLAS, HTR, IMPORTANCE SAMPLING, FAILURE, FUEL PARTICLE.

N° EOTP

A-SCRCG-09

En l'absence d'accord ou de contrat, les informations contenues dans le présent document ne sont pas destinées à la publication. Il ne peut en être fait état sans autorisation expresse du Chef de Service.

	Nom	Visa	Date	Classification				
Assurance Qualité	G. ARÈNE		12/09/06	Lib	DR	CC	CD	SD
Approbateur	P. OBRY		30/08/05	X				
Vérificateur	M. PHELIP		22/08/2005	Cadre de réalisation du document				
Rédacteur	F. MICHEL		05/08	HTR-F WP3				



RÉVISIONS

DATE	OBJET DES RÉVISIONS	INDICE
July 2005	Emission initiale.	0



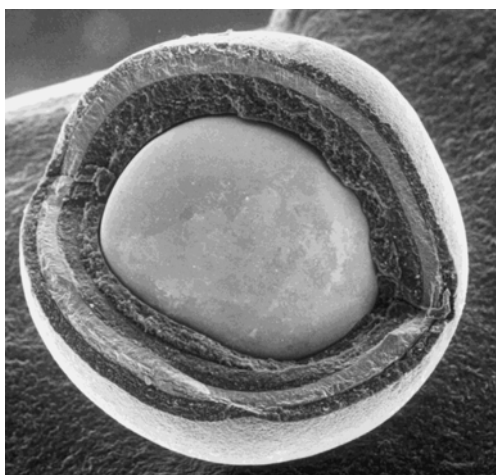
SOMMAIRE

1. INTRODUCTION	4
2. INPUT DATA FOR CALCULATION	4
3. MEAN PARTICLE BEHAVIOR	6
4. MEAN FAILURE FRACTION CALCULATION METHODS.	12
4.1. FAILURE PROBABILITY OF ONE PARTICULE	12
4.2. PREVIOUS STUDY	12
4.3. IMPORTANCE SAMPLING METHOD.	13
4.3.1. Theory	13
4.3.2. Application	14
4.4. POLYNOMIAL APPROCH	16
5. STATISTICAL RESULTS	18
5.1. FAILURE FRACTION	18
5.2. EVENTUAL HEATING TEST RESULTS	19
5.3. SENSIBILITY TO THICKNESS VARIATION AND VARIANCE	20
6. CONCLUSION	21
RÉFÉRENCES	22
LISTE DES ANNEXES	24

1. INTRODUCTION

This document constitute the deliverable n°3-2 of the HTR-F1 European project. In parallel to this work made in the work-package 3 (fuel modelling) of the HTR-F1 project, Dr. Nabielek invited (annex B) the world-wide teams working on HTR simulation codes to do the simulation of HFR EU1 experiment in order to compare the results. The basis data to do the simulation can be found in doc [4].

The HFR EU1 experiment will start in the years 2005 at high flux reactor of the European Commission (HFR) in Petten. The particles should reach about 20% FIMA for a fast fluence (>0.1 MeV) about 6.10^{25} neutrons/m²/s.



The “TRISO” HTR particle used in this irradiation is composed by a UO₂ fuel kernel surrounded by a porous pyrocarbon layer (buffer), an inner pyrocarbon dense layer (IPyC), a silicon carbide layer (SiC) and a outer PyC layer (OPyC). This layers form a tiny pressure vessel that must retain all fission products. The SiC layer is the most impervious layer to fission products and so we worry particularly about the failure fraction of the SiC layer.

The failure of the SiC layer can be led by SiC corrosion, PyC failure, asphericity defaults or pressurization. In this study, we consider a perfect spherical fuel, with only internal pressure as a cause of SiC layer failure.

2. INPUT DATA FOR CALCULATION

We use WP3 European HTR-F project recommendations, which are summarised in documents [1] and [2]. In those properties, we will use 3 different sets of data to study the behaviour of the particle and calculate corresponding failure fraction. In the ATLAS code, they are under the following material names :

	"BNFL"	"CEGA"	"FZJ"
Kernel	UO2_HTRF		UO2_HTRF
	Without creep as recommended in [3]		
Buffer	BuFFBNFL	BuFFCEGA	BuFF_FZJ
	With young modulus decreased by an factor of ten		
IpyC	PyC_BNFL	PyC_CEGA	PyC_FZJ
SiC	SiC_BNFL	SiCb_CEA	SiC_FZJ
OPyC	PyC_BNFL	PyC_CEGA	PyC_FZJ

The simulated particle is spherical with, at initial condition (for a fabrication temperature of 1500K), no gap between the layers, no stress and with the given layer thicknesses of document [4] which are :

Kernel diameter	$502.2 \pm 10.8 \mu\text{m}$
Buffer thickness	$94.9 \pm 14.3 \mu\text{m}$
IPyC thickness	$41.0 \pm 3.4 \mu\text{m}$
SiC thickness	$35.4 \pm 1.9 \mu\text{m}$
OPyC thickness	$40.0 \pm 3.8 \mu\text{m}$

The particle is spherically loaded. We define the 5 following phases :

- Decrease of the temperature from 1500K to ambient (300K) in 1000 s
- Temperature increase to nominal temperature (1223 K or 1373 K) in 10000s under increasing neutron flux
- unchanged nominal conditions until we reach the 600 days of irradiation ($5,184.10^7\text{s}$).
- Decrease to 300 K with no neutron flux in 10000s
- Heating to the temperature of 1500K to 1900K, in order to simulate a potential heating test, after irradiation.

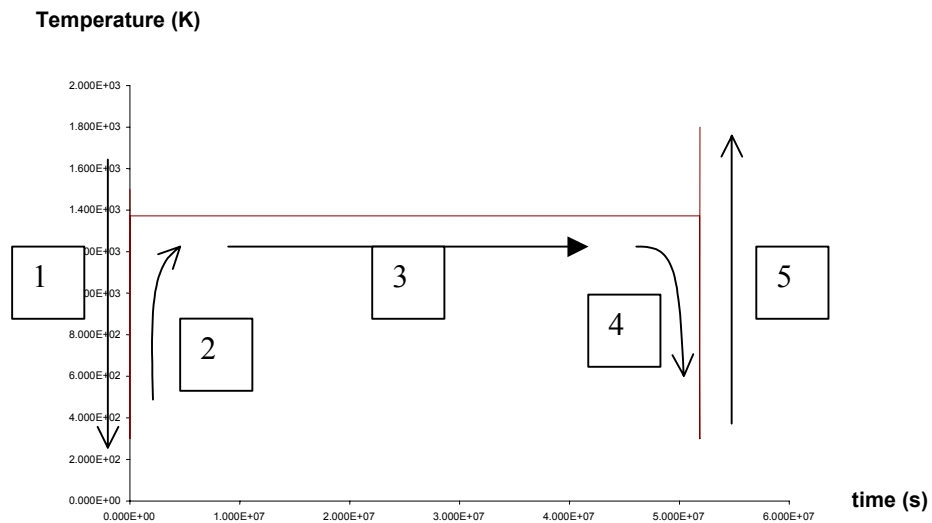


FIGURE 1: EXTERNAL IMPOSED TEMPERATURE HISTORY.

The imposed external pressure is always 0.1 MPa.

We give on the page 25 the ATLAS input data file for the case with “BNFL” properties and irradiation at 1223K.

3. MEAN PARTICLE BEHAVIOR

Due to the difference in thermal expansion between PyC and SiC, there is, at room temperature, a tensile stress created in SiC layer, proportional to temperature decrease after fabrication.

When irradiation experiment begin, the preceding stress is lowered. Note that if we had considered a initial temperature lower than irradiation temperature, the temperature increase would imply a contact between the kernel and the layers which would create an important stress in the SiC layer.

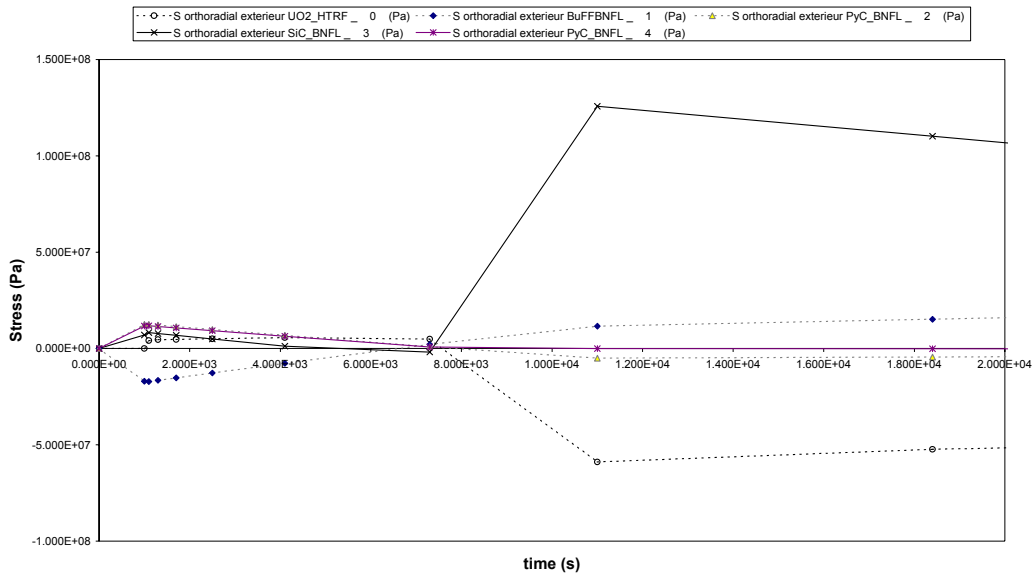


FIGURE 2 : CIRCUMFERENTIAL STRESS AT BEGINNING OF LIFE FOR A FABRICATION TEMPERATURE OF 1000K

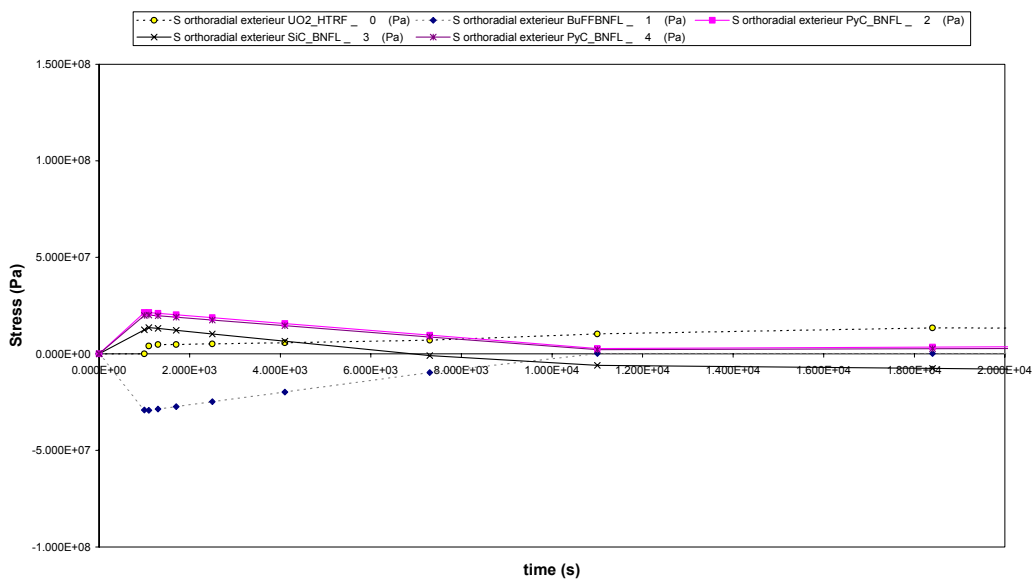


FIGURE 3 : CIRCUMFERENTIAL STRESS AT BEGINNING OF LIFE FOR A FABRICATION TEMPERATURE OF 1500K

Under irradiation, the Buffer shrinks and (we suppose so in ATLAS) debonds from IPyC. The PyC shrinkage produces a compressive stress in SiC layer. This stress stabilizes at equilibrium between shrinkage rate and irradiation induced creep of PyC.

Due to the creation and release of fission product gases, the internal pressure increase slowly and make the stress in SiC raise and become positive. This can lead to the failure.

After irradiation (or during irradiation), the temperature decrease do not generate tensile stress in SiC layer or gas release and so do not lead to rupture.

The heating test has the contrary effect : it raises the gas release and the internal gas pressure even at release rate constant.

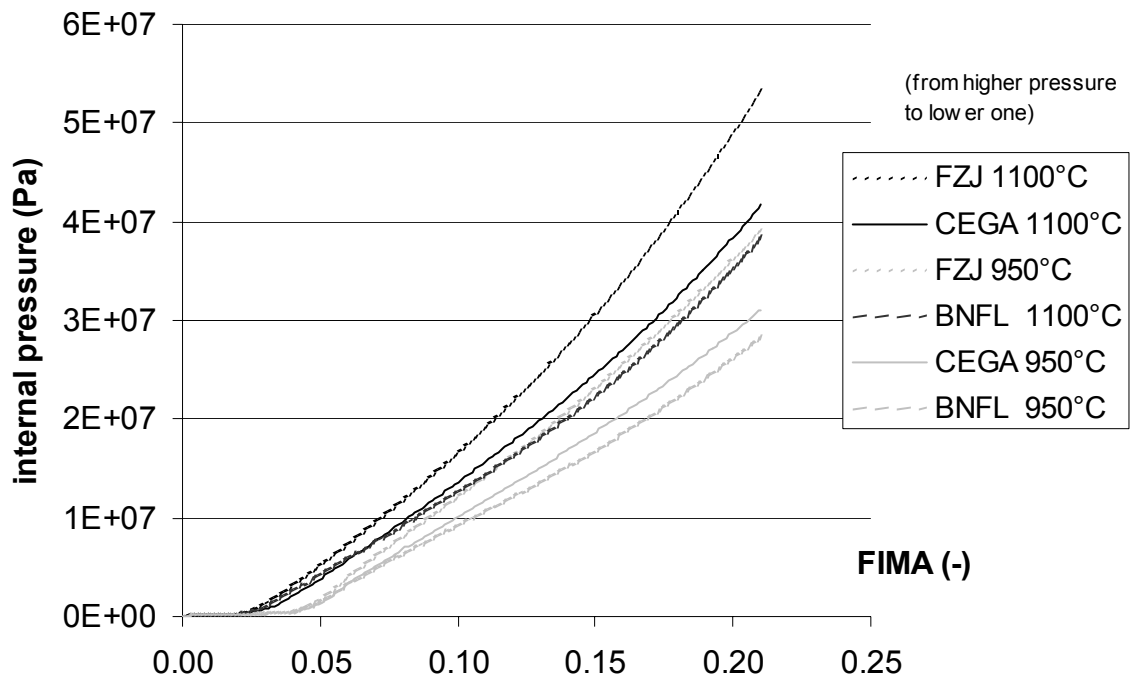
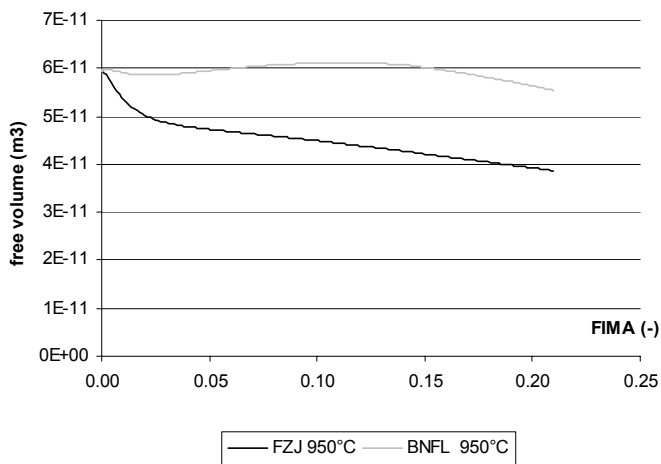
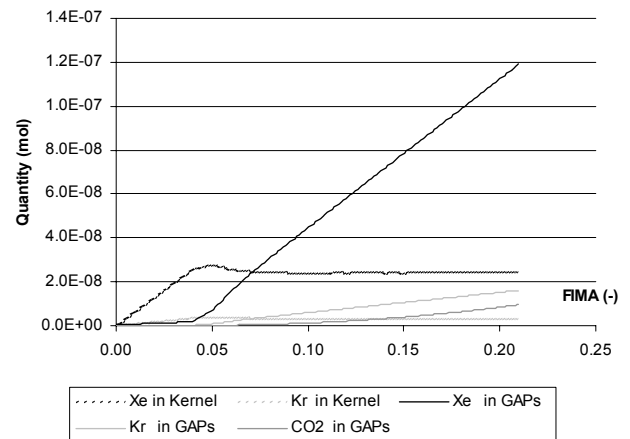


FIGURE 4 : EVOLUTION OF INTERNAL PRESSURE FOR THE 6 MEAN PARTICLE SIMULATION

FIGURE 5 :EVOLUTION OF FREE VOLUME
(THE DIFFERENCE IS DUE TO IPYC SHRINKAGE)FIGURE 6 :EVOLUTION OF GAS QUANTITY PRODUCED AND
RELEASED BY THE KERNEL AT 950°C.

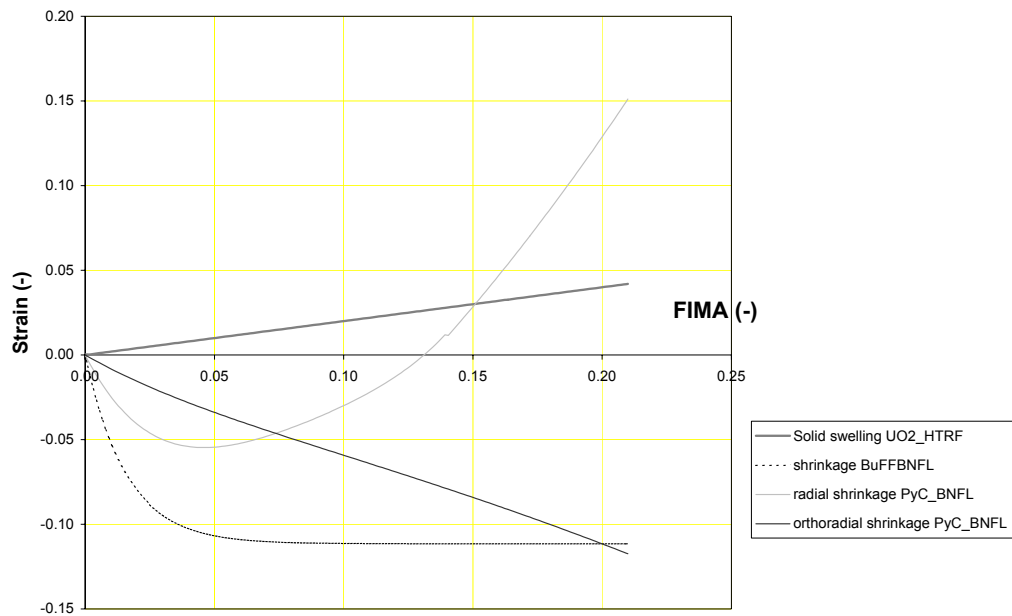


FIGURE 7 : IRRADIATION INDUCED DIMENSIONAL CHANGES FOR "BNFL" LAWS

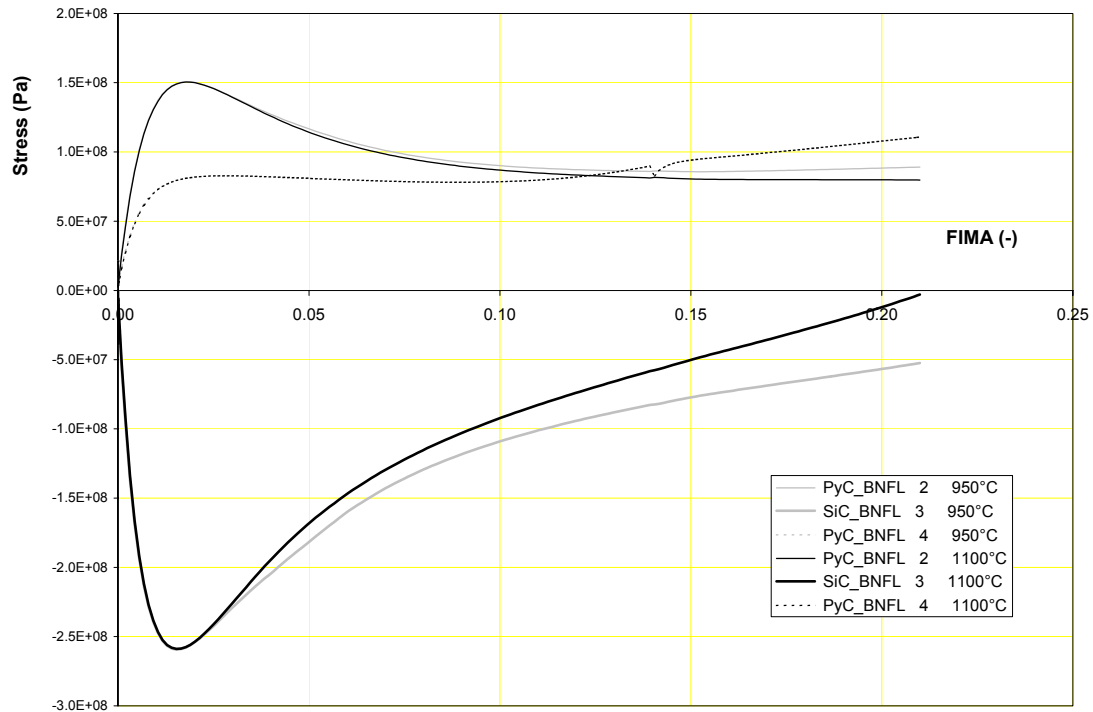


FIGURE 8 : OUTER SKIN CIRCUMFERENTIAL STRESS IN THE LAYERS FOR "BNFL" LAWS CALCULATION

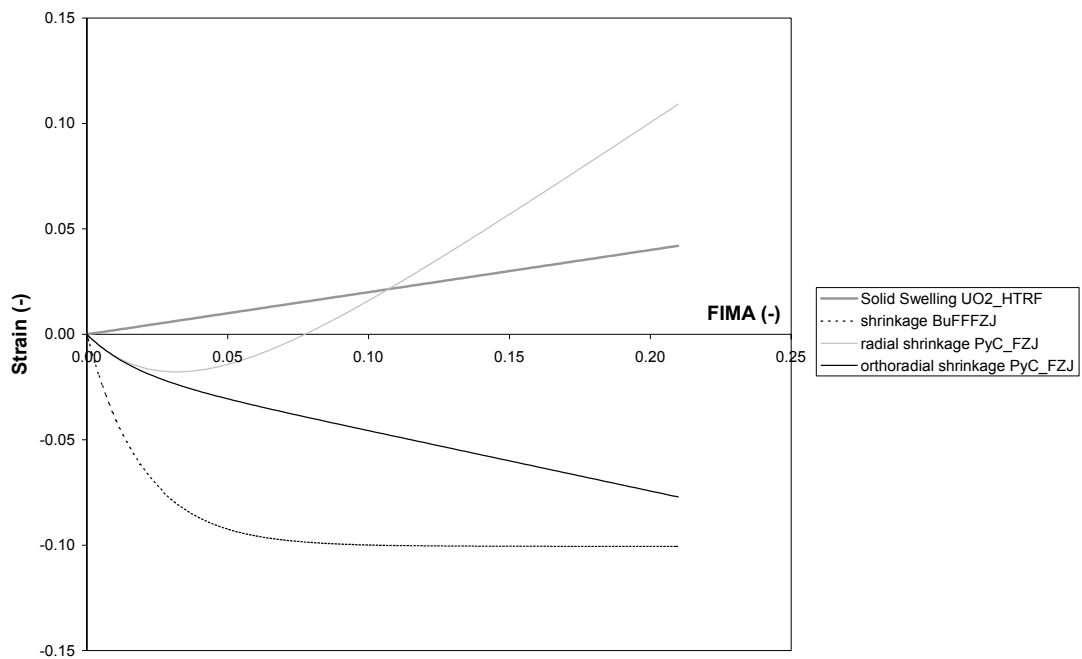


FIGURE 9 : IRRADIATION INDUCED DIMENSION CHANGES FOR "FZJ" LAWS

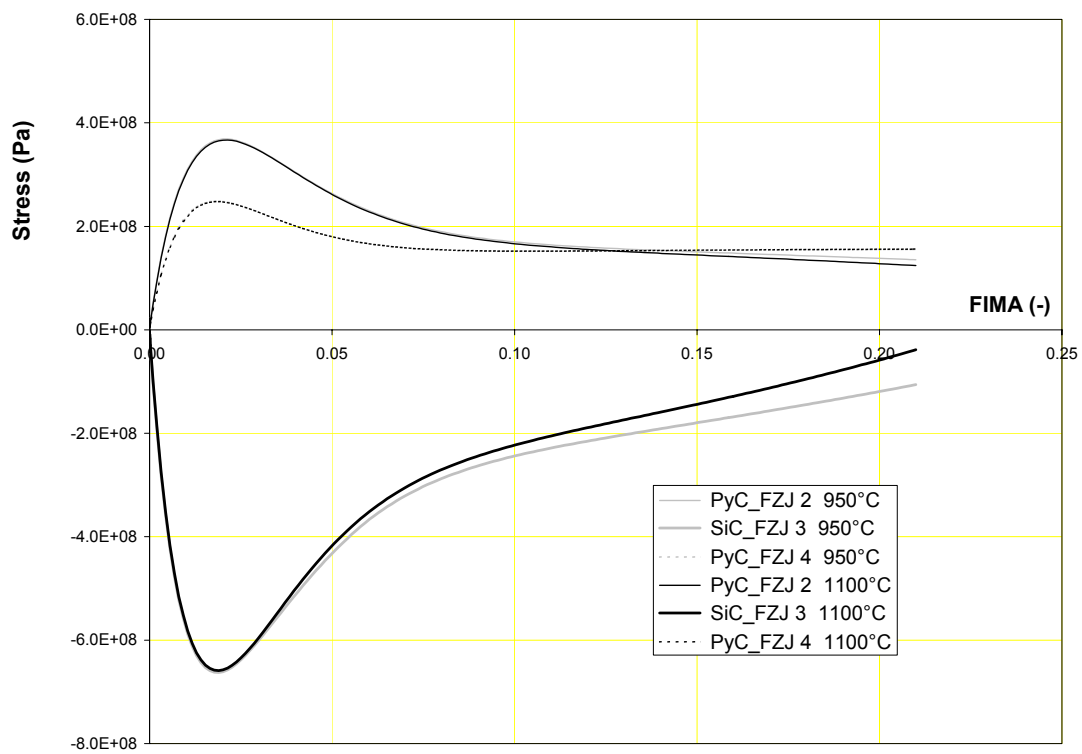


FIGURE 10 : OUTER SKIN CIRCUMFERENTIAL STRESS IN THE LAYERS FOR "FZJ" CALCULATION

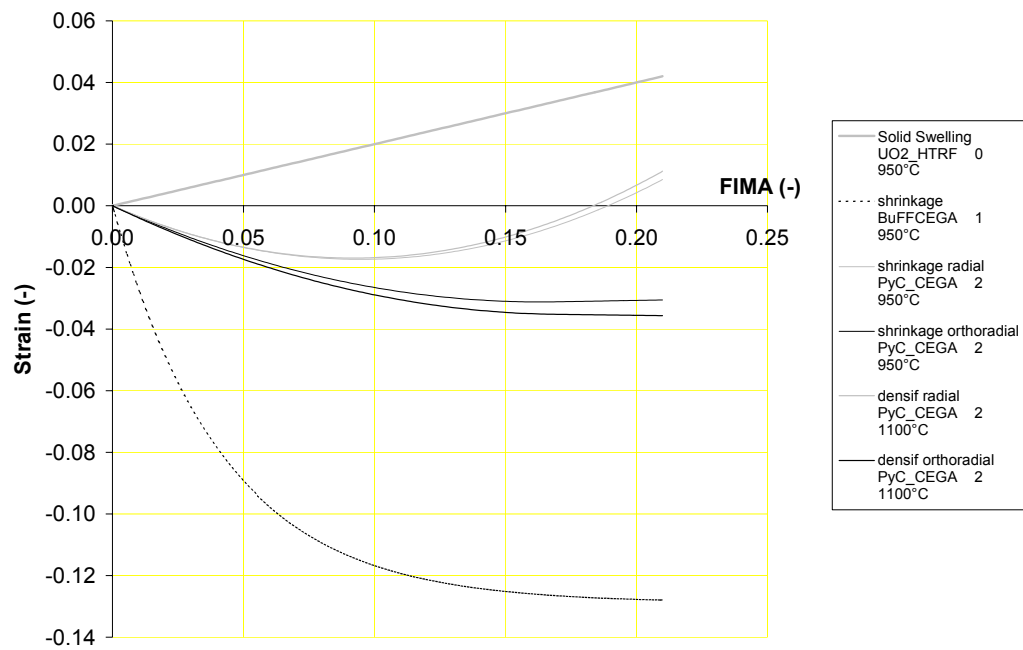


FIGURE 11 : IRRADIATION INDUCED DIMENSION CHANGES FOR "CEGA" LAWS

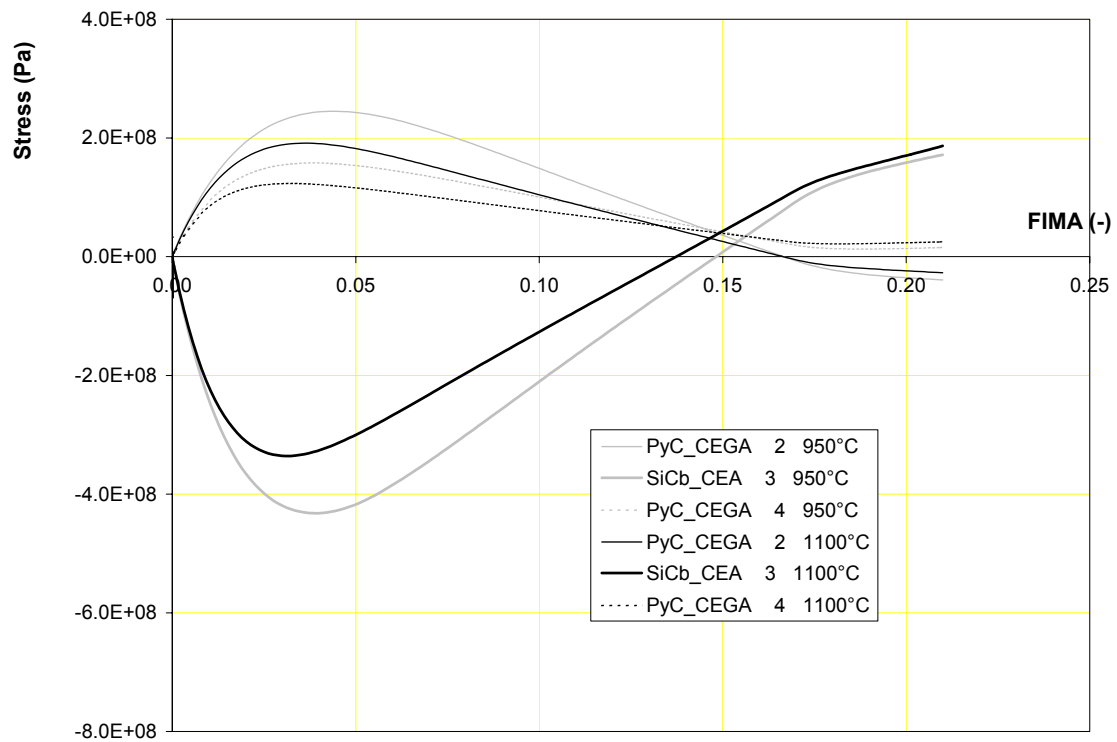


FIGURE 12 : OUTER SKIN CIRCUMFERENTIAL STRESS IN THE LAYERS FOR "CEGA" CALCULATION

4. MEAN FAILURE FRACTION CALCULATION METHODS.

4.1. FAILURE PROBABILITY OF ONE PARTICULE

We consider that failure probability can only be due to tensile stress in SiC layer, with no PyC layer defect or failure. This happens when the maximum tensile stress in SiC exceed the given strength of the layer. The strength of the SiC layer follow a Weibull law probability function. So, the probability of failure P is given by the function :

$$P(\sigma) = 1 - e^{-\ln 2 \left(\frac{\sigma}{\sigma_m} \right)^m}$$

where σ is the maximum tensile stress in SiC layer and σ_m and m are given independently of the stress profile and SiC layer thickness . For them, we take the function of fluence at 1100°C from doc [5] i.e. the following function of the time t (in s) :

$$\sigma_m = 10^6 \cdot \left(834 - 57.1 \frac{f_{end}}{t_{end}} t \right) \quad (\text{Pa})$$

$$m = 8.02 - 0.425 \frac{f_{end}}{t_{end}} t \quad (-)$$

with an irradiation time $t_{end} = 5.18 \cdot 10^7$ s

and a fast fluence $f_{end} = 6$ (in 10^{25} neutrons/m²)

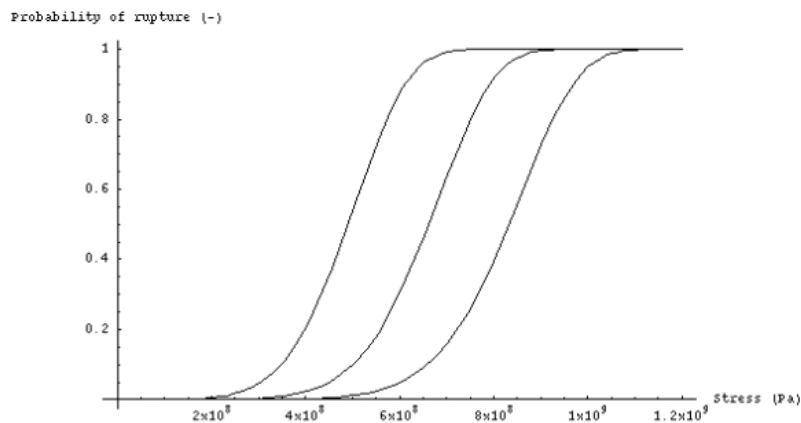


FIGURE 13 : SiC FAILURE PROBABILITY IN BEGIN (RIGHT CURVE), MIDDLE AND END (LEFT CURVE) OF IRRADIATION AS A FUNCTION OF MAXIMUM TENSILE STRESS OF THE LAYER.

4.2. PREVIOUS STUDY

The simplest statistical method to determinate the mean failure fraction of the particles is the Monte-Carlo method.

In a previous study (Ref ¹), we made a crude¹ monte carlo with 100 simulations and noticed that it was not representative of the mean failure probability. More precisely we noticed that :

- The majority of the contribution to mean failure probability is due to particle very different to the mean particle.
- The buffer thickness is the most important geometric parameter on failure probability. Very low buffer thickness lead to high failure probability.

As the tail of the buffer thickness distribution is of higher importance than the failure probability function, we will need a large number of calculations to have an accurate result.

In the following, we will use two methods derivative to Monte Carlo, and we will focus on low buffer thickness particles.

4.3. IMPORTANCE SAMPLING METHOD.

4.3.1. Theory

We have to determine the mean value of the failure probability of the particle :

$I = \int g(x)dF(x)$ Where I is the mean failure probability, g(x) is the failure probability of one particle and dF(x) the density of the distribution F of the particles.

With monte-carlo, we would use the equality : $\hat{I} = \frac{1}{n} \sum_{\text{sample of n particle following F distribution}} g(X_i) \xrightarrow{n \rightarrow \infty} I$

The importance sampling method introduce a function $\tilde{f}$ and use the equality :

$$I = \int \frac{f(x).g(x)}{\tilde{f}(x)} \tilde{f}(x).dx$$

so I can be estimated :

$$I \approx \frac{1}{n} \sum_{\text{sample of n particle following } \tilde{F} \text{ distribution}} \frac{f(x_i).g(x_i)}{\tilde{f}(x_i)}$$

Note that we must have $\tilde{f}(x) > 0$ everywhere where $f(x) > 0$.

The goal is to determine a distribution which decreases the variance of the estimate. There are some good methods to approach this best function. We don't use them here. Let's say that a good function will build a sample concentrated where the product $g(x)*f(x)$ is maximum.

¹ Contrary to « hit or miss » Monte Carlo in which we count the failures on a sample, in the crude Monte-Carlo we separate one parameter which lead to failure (here the SiC strength) and calculate the mean of this function response on the sample.

4.3.2. Application

In our case, we saw that the contribution to failure fraction, that is the product failure probability by the density of occurrence is maximum for particles with buffer thickness under 70 microns. This result depends on the calculation and on the time taken into account, but we have chosen to keep an importance distribution centred on this value. We took a dispersion bright enough to include initial distribution in taking the double standard deviation. Without any study of others parameter influence, we kept for them a distribution centred on mean value but used double standard deviation for all layers.

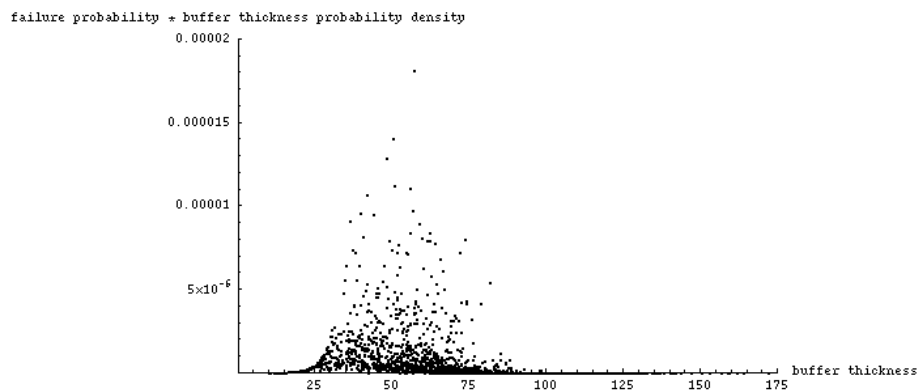


FIGURE 14 : "IMPORTANCE" OF LOW BUFFER THICKNESS PARTICLE AT END OF IRRADIATION FOR "BNFL" PROPERTIES

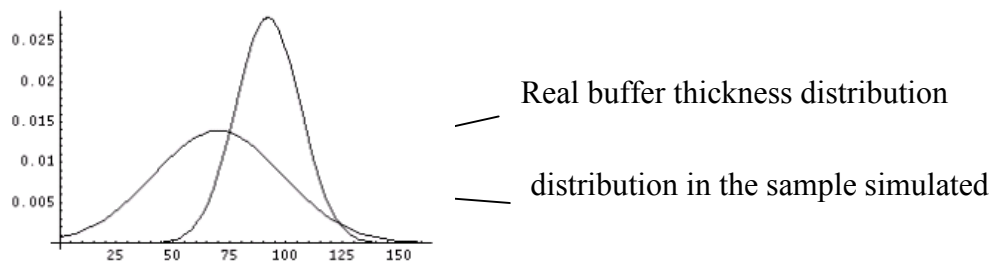


FIGURE 15 : REAL AND SIMULATED DISTRIBUTIONS OF BUFFER THICKNESS

We took gaussian distributions for the thicknesses of the layers (diameter of kernel) defined by the mean values = {502.2, 70., 41, 35.4, 40} and the standard deviation = {10.8, 28.6, 6.8, 3.8, 7.6}.

As the ATLAS code cannot handle with negative or near zero buffer thickness, we used a truncated distribution in keeping only buffer thicknesses > 10 microns. Excluded particles represents 1,8% of the sampling, so it was taken into account in the value of the importance function density $\tilde{f}$ in the mean calculation. The probability for the initial buffer distribution to reach lower values is only $6.3 \cdot 10^{-10}$ and so, not represented particles could be neglected.

We made 2000 simulations in the case "BNFL" at 1100°C.

The sample buffer thickness as the following distribution :

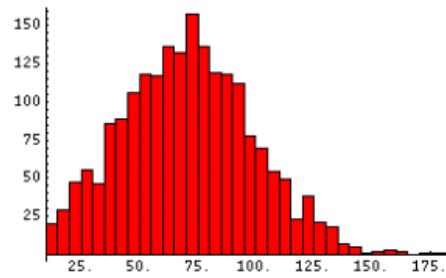


FIGURE 16 : EFFECTIVE DISTRIBUTION OF BUFFER THICKNESS IN THE SIMULATED SAMPLE

For each particle in the sample, we made the corresponding numerical simulation with ATLAS V1.0 and we obtained the circumferential stress in SiC layer as a function of time, at inner skin, where the stress is maximum.

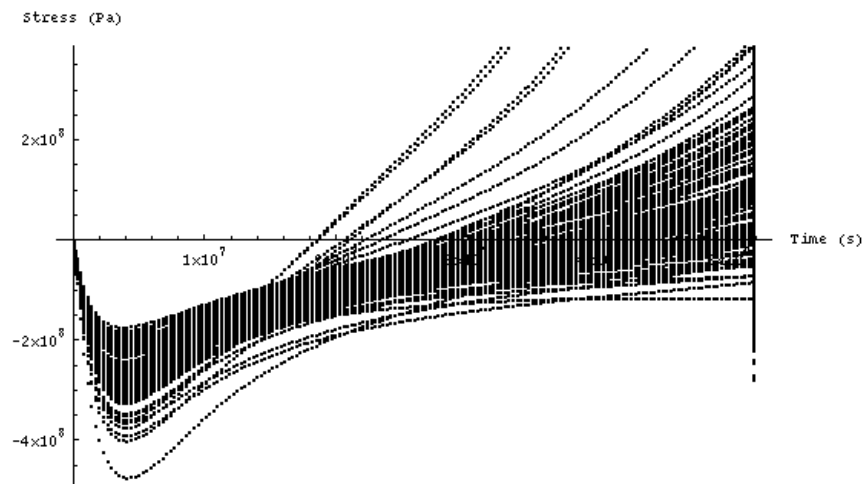


FIGURE 17 : EVOLUTION OF CIRCUMFERENTIAL STRESS IN SiC FOR THE FIRST 100 SIMULATION FOR BNFL CASE AT 1100°C.

All simulation ended without error.

We calculated the mean failure probability on the 4 different sub-samples of 500 particles each, to have an evaluation of the error.

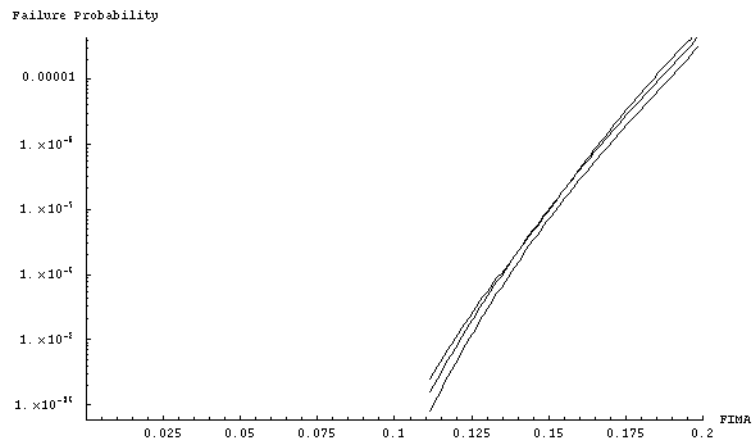


FIGURE 18 : MEAN FAILURE PROBABILITY FOR 4 DIFFERENTS SERIES OF 500 PARTICLES (2 ARE STACKED)

We notice an error between different batches which reach 50% of the value. This relative error does not increase significantly for very low probability. Regarding the high uncertainty due to the behaviour, this error can be considered low and this method is easier to use than the following.

4.4. POLYNOMIAL APPROCH

For each time step separately, we will find the polynomial that will best fit the results of the ATLAS code.

By plotting the results of the code on the 2000 random particles, we noticed that the buffer influence look like an $1/x$ curve.

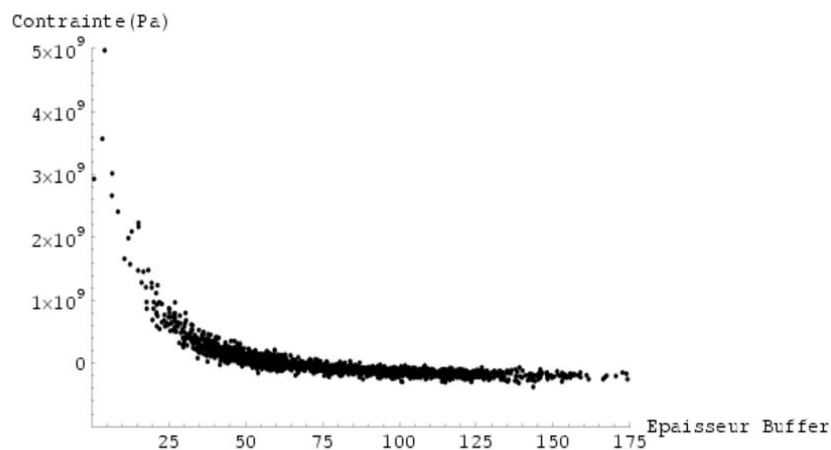


FIGURE 19 : STRESS IN SiC OVER BUFFER THICKNESS.FOR RANDOM PARTICLES

For that reason we tried to adjust the polynomial on the result of the code as a function of the inverse of the layer thickness. We can plot at one time for example, the 2000 results obtained by the code and those obtained by the polynomial regression of the 1000 first simulations. We verified that the regression made on the inverse of the layer thickness was much better than the one on the thickness value.

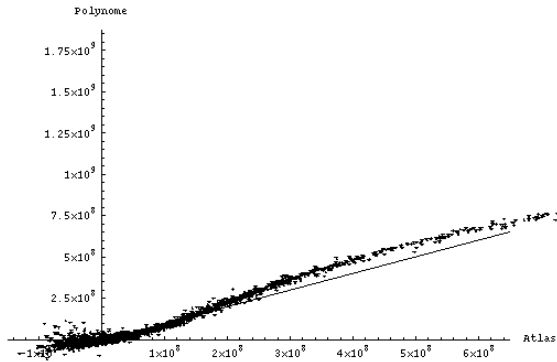


Figure 20 :

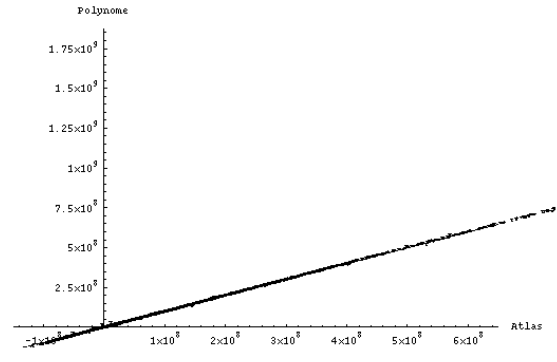


Figure 21 :

Comparison of the stress value obtained by ATLAS code and those obtained with a 3rd order fitting polynomial of

the layer thickness

the inverse of layer thickness

The second step of this method is to calculate the mean failure probability with particle behaviour given by the polynomial. This could be done by direct integration but it was easier to do a Monte Carlo like estimation of the mean failure probability. For this step, we used an importance sampling method, with the same importance distribution function than above. With 10^6 random particles, the error becomes low, as it is shown here :

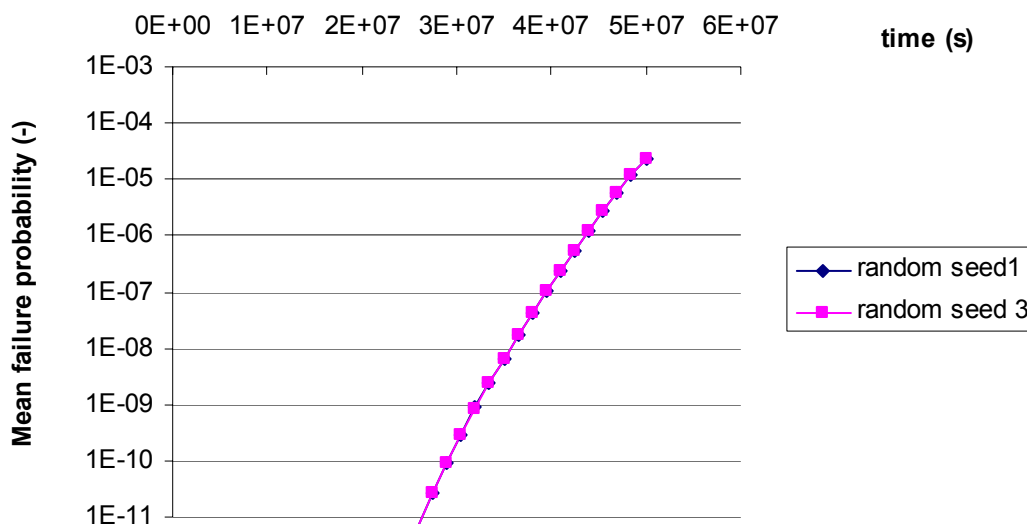


FIGURE 22 : CALCULATION BY IMPORTANCE SAMPLING METHOD OF THE PARTICLE MEAN FAILURE PROBABILITY WITH THE STRESS GIVEN BY A 3RD ORDER POLYNOMIAL, WITH 10^6 RANDOM PARTICLES.

The principal error should be to approximate the code behaviour by a polynomial, for two reasons : the polynomial adjustment should be bad (here we have an excellent adjustment : $RSquared = 0.9997$) or the sample should be too small to be representative. To have a chance to estimate the error at this step, we made 4 estimations of the mean failure probability, based on the 4 quarters of the 2000 simulations we did. We found a very low variation of the results.

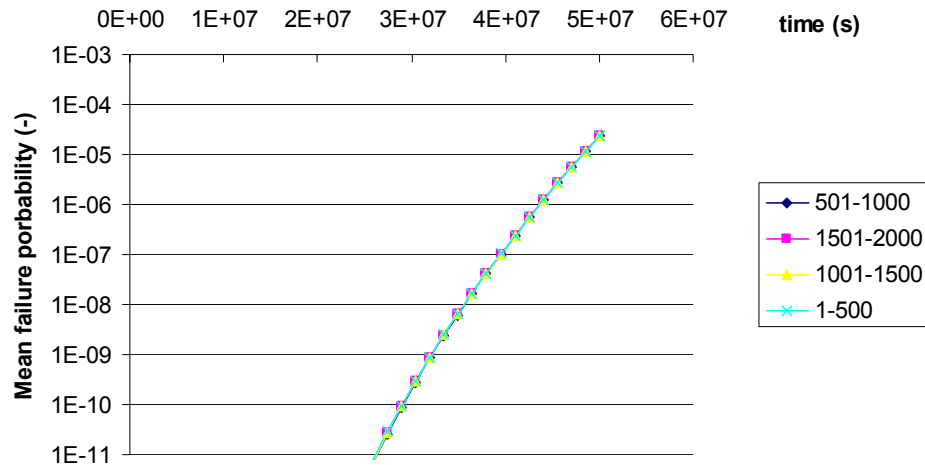


FIGURE 23 : MEAN FAILURE PROBABILITY CALCULATED THROUGH THE USE OF A FITTING 3RD ORDER POLYNOMIAL OF 4 DIFFERENTS RANDOM BATCHES OF 500 PARTICLES.

So, we suppose that we have a good estimation of the mean failure probability given by the ATLAS simulation.

5. STATISTICAL RESULTS

5.1. FAILURE FRACTION

We used the polynomial regression of the ATLAS results to determine the mean failure probability for each of the 6 cases we wanted to study (3 batches of properties, 2 temperatures). For this, we made 400 ATLAS simulations in each case.

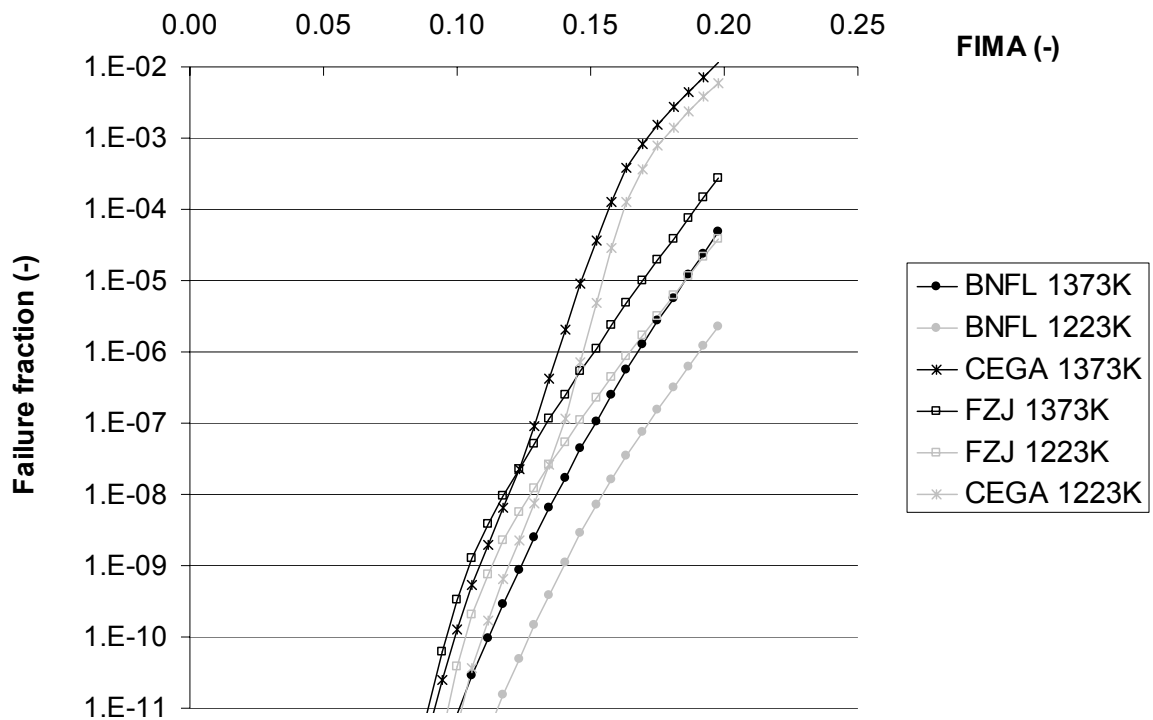


FIGURE 24 : MEAN FAILURE PROBABILITY FOR SPHERICAL PARTICLES IN HFR-EU1 EXPERIENCE FOR DIFFERENT LAW BATCHES.

Probability increasing very quickly, we have to consider the logarithm of the failure fraction or the time at which we reach one specific failure fraction. We resume the results in this form in the table below :

	10 ⁻⁶ not measurable	10 ⁻⁵	10 ⁻⁴ surely measurable
BNFL 1223 K	19	~21	~24
BNFL 1373 K	17	18.5	20
CEGA 1223 K	15	15.5	16
CEGA 1373 K	14	14.5	16
FZJ 1223 K	16.5	18.5	20
FZJ 1373 K	15	17	19

According to ATLAS with use of BNFL or FZJ properties, there will be very few particle failures during irradiation occurring (if any) near the end of irradiation time.

5.2. EVENTUAL HEATING TEST RESULTS

If we realise an heating test on the particles after HFR-EU1 experiments, we should obtain the following particle mean behaviour :

	Failure fraction for a heating test when reaching the temperature :				
	1500 K	1600 K	1700 K	1800 K	1900 K
FZJ (1223K)	$1.76 \cdot 10^{-5}$	$7.95 \cdot 10^{-5}$	$0.19 \cdot 10^{-3}$	$0.37 \cdot 10^{-3}$	$0.68 \cdot 10^{-3}$
BNFL (1223K)	$0.16 \cdot 10^{-3}$	$0.57 \cdot 10^{-3}$	$1.06 \cdot 10^{-3}$	$1.6 \cdot 10^{-3}$	$2.45 \cdot 10^{-3}$

By doing calculation at diverse temperature, we show here a dependence to the temperature reached. The particle should here have a significant failure rate.

5.3. SENSIBILITY TO THICKNESS VARIATION AND VARIANCE

The advantage of importance sampling based methods is that simulation results for a given population can be used to determine the statistical behaviour of another population (with entry parameters following an other distribution). It corresponds by changing the f function in the sum calculation in §4.3.1. So, we didn't need to make further simulations.

We present here some parameter change influences :

Calculation done from a basis "BNFL" at 1373 K	Final failure fraction
Basis	$4.6 \cdot 10^{-5}$
Buffer thickness dispersion * 2	$1.7 \cdot 10^{-2}$
Buffer thickness dispersion / 2	$4.6 \cdot 10^{-7}$
Buffer thickness = 100 μm (+5 μm)	$1.43 \cdot 10^{-5}$
SiC thickness = 40 μm (+5 μm)	$2.67 \cdot 10^{-5}$
SiC thickness dispersion * 2	$5.48 \cdot 10^{-5}$
Kernel diameter dispersion * 2	$4.6 \cdot 10^{-5}$
Dense PyC thickness dispersion * 2	$6 \cdot 10^{-5}$
Initial strength for SiC during all irradiation	$6.1 \cdot 10^{-7}$

The buffer appears here to be the most important parameter. Controlling its distribution (and we can guess its sphericity) is a key point for obtaining a good particle behaviour at 20% FIMA.

The SiC strength is another important parameter. If it does not decrease during irradiation, the probability to have one failure before the end of irradiation becomes low.



6. CONCLUSION

The particle behaviour in the HFR-EU1 experiment according to ATLAS is classical : the internal pressure increase and counter balance the shrinkage of PyC compression of the SiC layer. Near the end of irradiation, SiC layer circumferential stress become positive.

In experiment HFR-EU1, we can obtain failures during irradiation, depending mostly on the thickness distribution of the buffer. With the given distributions and strength distribution, the particle failure rate increase very fast and so, the first particles failure due to irradiation will be followed quickly by many others. We can expect a failure rate between 0 ($\leq 10^{-5}$) and 10^{-3} .

A post irradiation heating test should give a more measurable results. Note that we did not take into account the defect of sphericity of the particles.



RÉFÉRENCES

- [1] PELLETIER M., NABIELEK H., ABRAM T. & MARTIN D. "HTR-F Project : Selection of properties and models for coated particle : PyC and SiC." NT SESC/LSC 03-028. Juin 2003.
- [2] MICHEL Frédéric « Description de la version V0.2 d'ATLAS et des lois des combustibles carbures utilisées » .NT DEC/SESC/LSC 03-023. Juillet 2003.
- [3] MICHEL Frédéric. « Notice d'utilisation d'AtlasV1.0 » NT SESC/LSC/03-039. Octobre 2003.
- [4] NABIELEK Heinz, VERFONDERN Karl & WERNER Heinz. „Selection of benchmark cases for mechanical failure prediction“ EC document HTR-F-0408-D-3.1
- [5] GOLUBEV I.E. « Calculational researches of the coated particles performance in normal operation conditions ». CEA/RRC KI cooperation on future systems. Report 1.3 Task 1.
- [6] TUFFERY Patrice. « Probabilités de rupture d'une particule TRISO ». Rapport de stage, université Paul Sabatier. Septembre 2003.

TABLE DES FIGURES

Figure 1: External imposed temperature history.	6
Figure 2 : Circumferential stress at beginning of life for a fabrication temperature of 1000K	7
Figure 3 : Circumferential stress at beginning of life for a fabrication temperature of 1500K	7
Figure 4 : Evolution of internal pressure for the 6 mean particle simulation	8
Figure 5 : Evolution of free volume (the difference is due to iPyC shrinkage)	8
Figure 6 : Evolution of gas quantity produced and released by the kernel at 950°C.	8
Figure 7 : irradiation induced dimensional changes for “BNFL” laws	9
Figure 8 : outer skin circumferential stress in the layers for “BNFL” laws calculation	9
Figure 9 : irradiation induced dimension changes for “FZJ” laws	10
Figure 10 : outer skin circumferential stress in the layers for “FZJ” calculation	10
Figure 11 : irradiation induced dimension changes for “CEGA” laws	11
Figure 12 : outer skin circumferential stress in the layers for “CEGA” calculation	11
Figure 13 : SiC failure probability in begin (right curve), middle and end (left curve) of irradiation as a function of maximum tensile stress of the layer.	12
Figure 14 : ”Importance” of low buffer thickness particle at end of irradiation for “BNFL” properties	14
Figure 15 : real and simulated distributions of buffer thickness	14
Figure 16 : Effective distribution of buffer thickness in the simulated sample	15
Figure 17 : Evolution of circumferential stress in SiC for the first 100 simulation for BNFL case at 1100°C.	15
Figure 18 : Mean Failure probability for 4 differents series of 500 particles (2 are stacked)	16
Figure 19 : Stress in SiC over buffer thickness, for random particles	16
Figure 20 : Comparison of the stress value obtained by ATLAS code and those obtained with a 3 rd order fitting polynomial of the layer thickness	17
Figure 21 : Comparison of the stress value obtained by ATLAS code and those obtained with a 3 rd order fitting polynomial of the inverse of layer thickness	17
Figure 22 : Calculation by importance sampling method of the particle mean failure probability with the stress given by a 3 rd order polynomial, with 10 ⁶ random particles.	17
Figure 23 : Mean failure probability calculated through the use of a fitting 3 rd order polynomial of 4 differents random batches of 500 particles.	18
Figure 24 : Mean failure probability for spherical particles in HFR-EU1 experience for different law batches.	19



LISTE DES ANNEXES

<i>Annexe A : fichier des données d'entrées pour ATLAS V1.0</i>	25
<i>Annexe B : Email Message from H.Nabielek</i>	26



ANNEXE A : FICHIER DES DONNÉES D'ENTRÉES POUR ATLAS V1.0

***** MAILLAGE

Type de maillage [mot cle' 1D , 2Dcentre ou 2D] de'faut 2D

'1D'

Nb de couches et couche etanche

4 2

rayon noyau (m) et nb de mailles suivant le rayon

0.0002511 9

Jeux entre couches (n-1) et n

1 1.E-7

2 1.E-7

epaisseur minimale des jeux entre couches (2.E-7 conseille') (m)

1.E-7

epaisseur couches (m) et nb de mailles dans l'epaisseur

94.9E-6 5

41.0E-6 4

35.4E-6 4

40.0E-6 4

nombres de portions divisant pi/2 radians du maillage spherique

12

*

***** MATERIAUX

Noyau : Materiau (mot) et porosite' (/)

UO2_HTRF 0.0082

Noyau : enrichissement , taille grains (m), stoech

0.1676 1.E-6 2.008

Fission : Energie et unite' et nb d'at de gaz produits (/)

200 MeV

Gaz atoms per fission : 'name' and rate (/)

'Xe' 0.265

'Kr' 0.036

Couches : mate'riau (MOT) et porosite' (/)

'BuFFBNFL' 0.5522

'PyC_BNFL' 0.1726

'SiC_BNFL' 0.00498

'PyC_BNFL' 0.1726

Taux d'ouverture des porosités

0.1 1.0

Gaz interne a` la particule de fabrication (mot cle':XE) et pression (Pa)

'Xe' 1.E5

***** conditions spe'ciales (voir notice)

AF1 0 '*=' 0.1

AF3 0 '*=' 0.1

YOUN 1 '*=' 0.1

BAF 2 '==' 1.02

BAF 4 '==' 1.02

* * *

***** additional outputs

YOUN INTERIEUR 3

OPF INTERIEUR 0

GARR INTERIEUR 0

* * *

***** l'historique d'irradiation *****

**** Pression exterieure (en Pa)****

1.E5

*** flu neutronique

1.157E+18 'n/m2/s'

*** proba de fission=d[FIMA]/dt (s-1)5.E-9

4.05E-09

*** Nombre de pas (autres que t=0), les valeurs au dela ne seront lues

12

**** temps max d'une iteration (s) et multipleur

300000. 2.

**** mode de calcul du flu neutronique : Mot cle' (PROP ou X)

PROP

**** Historique t (s), evolution norme'e de la proba de fission

0. 1500.

1000. 300. 0.

1100. 300. 1.

11000. 1223. 1.

51841000. 1223. 1.

51841100. 1223. 0.

51851000. 300. 0.

51852000. 300. 0.

51853000. 1500. 0.

51853100. 1600. 0.

51853200. 1700. 0.

51853300. 1800. 0.

51853400. 1900. 0.



ANNEXE B : EMAIL MESSAGE FROM H.NABIELEK

Heinz Nabielek <heinznabielek@mac.com>

05/13/03 01:40 PM

To: he.werner@fz-juelich.de, Dr David G Martin

<martin@63foliat.freemove.co.uk>, PTI@inel.gov, k.verfondern@fz-juelich.de

cc: Michael Fütterer <michael.fuetterer@jrc.nl>, PHELIP DEC/SESC/LIAC

<PHELIP@drncad.cea.fr>, PELLETIER DENCAD-DEC-SESC

<PELLETIER@drncad.cea.fr>, GUILLERMIER Pierre <pguillermier@framatome.fr>

Fax to:

Subject: HFR-EU1 failure prediction

Dear Heinz, David (Martin) and David (Petti), and Karl:

we would like to invite you to an early
attempt at HFR-EU1 failure prediction:

irradiation

20% FIMA in 600 full power days reaching
36e20 neutrons pro cm2 (EDN),
linear progress assumed even though
not quite correct for burnup

prediction for 4 cases

- (i) 1100°C with kernel-coating mechanical interaction
- (ii) 1100°C without kernel-coating mechanical interaction
- (iii) 950°C with kernel-coating mechanical interaction
- (iv) 950°C without kernel-coating mechanical interaction

UO2 kernel

diameter 502.2 um

diameter sdev 10.8 um



swelling 0.8 percent per percent fima

98% theoretical density

buffer layer

thickness 94.9 um

thickness sdev 14.3 um

46% theoretical density (from 2.2)

iPyC layer

thickness 41.0 um

thickness sdev 3.4 um

85% theoretical density (from 2.2)

anisotropy 1.02

SiC layer

thickness 35.4 um

thickness sdev 1.9 um

99.5% theoretical density (from 3.216)

Ultimate Tensile Strength

median 834 MPa, or 8181 kp/cm²

m=8.02

oPyC layer

thickness 40.0 um

thickness sdev 3.8 um

85% theoretical density (from 2.2)

anisotropy 1.02



Can you make a quick prediction?

We want to discuss the consequences
next Monday at the WP2 meeting in Petten.

Eventually we will need to compare
more details like Xe, Kr pressure,
CO pressure, SiC weakening and corrosion.

For the moment, I suggest to use what the
present defaults are.

Best greetings

Heinz