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## High-Temperature Reactor Fuel Technology

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# HTR-F Project – WP3 – Deliverable n°13

# ATLAS first calculations

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SERVICE D'ETUDES ET DE SIMULATION DU COMPORTEMENT DES COMBUSTIBLES

LABORATOIRE DES IRRADIATIONS AVAL DU CYCLE

# HTR-F PROJECT - DELIVERABLE N°13
# ATLAS FIRST CALCULATIONS

DE G. DEGENEVE

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Titre : HTR-F PROJECT - DELIVERABLE N°13
ATLAS FIRST CALCULATIONS

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Résumé :

This document is the deliverable n°13 of the HTR-F project, Work-Package 3, Fuel Modeling. Its purpose is to present the first calculations performed with the European ATLAS code under development at the CEA/DEN/DEC/SESC/LSC. The aim of the ATLAS code is to simulate the in pile behavior of an HTR type fuel, namely a fuel whose basic element is a spherical particle.

The behavior laws and material characteristics were defined within a European framework. Concerning the layers, in addition to a simplified reference set, two sets of laws are used : a set from the BNFL English company and a set from the FZJ German research organization.

The thermal and mechanical evolutions of the particle under irradiation is a multi-parameter and complex phenomenon. The different sets of laws used led to rather different results, both in terms of stress and temperature.

Thus, it appears that it is important to be able to characterize :
- The deformation kinetics under fast flux of the pyrocarbon layers, particularly at the beginning of irradiation,
- The irradiation induced creep coefficient of the PyC layers, but also that of the SiC layer.
- The failure modes of the layers.
- The behavior of the buffer.

Increasing the knowledge on these PyC and SiC layer properties will be an important step for the design and understanding of the in pile behavior of future fabrications. This involves a fine re-interpretation of past experiments and carrying out experiments on analytical irradiations on materials elaborated under the same conditions as those of future fabrications.

| Mots Clés | HTR - ATLAS - HFR-P4 - FUEL |
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# 1. INTRODUCTION

This document is the deliverable n°13 of the HTR-F project, Work-Package 3, Fuel Modeling. Its purpose is to present the first calculations performed with the ATLAS code *[1]*, under development at the CEA/DEN/DEC/SESC/LSC.

The aim of the ATLAS code is to simulate the in pile behavior of an HTR type fuel, namely a fuel whose basic element is a spherical particle. The order of magnitude of the particle size is the mm. The particle consists of a fuel kernel embedded in several ceramic material layers.

The ATLAS module should be able to conduct :

- Thermal and mechanical deterministic calculations on a loose particle,
- Diffusion calculations on gaseous and metallic FPs through the particle layers,
- Calculations of fuel elements of compact or pebble type,
- Probabilistic calculations so as to estimate the probabilities of rupture of the layers during an experiment or even in a whole core using former calculations.

This document presents a deterministic thermal and mechanical calculation on a loose particle using the ATLAS code in its V1.0 version.

The calculation case corresponds to the HFR-P4 experiment, conducted at the beginning of the 80s. This experiment is relatively well documented (see §2.1). The calculations were made using updated material properties (see §2.2 and §2.3).

Using a set of reference material properties, additional calculations were made by changing a few parameters to measure their influence on the particle behavior.

# 2. BASIC DATA

## 2.1. GENERAL POINTS

The HFR-P4 experiment was irradiated 351 EFPD in HFR, from 06/10/82 to 11/28/83. A detailed report (réf.[2]) describes the fabrication, irradiation and post-irradiation examinations of this experiment. The objective of HFR-P4 was to test particles in a little pebble representative of a standard pebble fabrication and to compare the respective performances of both types of particles with two different SiC thicknesses (36 and 51 µm, see Figure 1). This experiment was conducted within a German framework for a small modular HTR 200 MWth « HTR-MODUL » and was aimed at exploring the limits of the low enriched uranium « triso » particle (LEU). Indeed, the nominal burnup for such a project was 9% FIMA and the irradiation temperature ranged from 700 to 900°C, whereas the HFR-P4 objectives were to reach about 15 % FIMA for an irradiation temperature greater than 900°C.

The irradiated objects were cylindrical compacts made of graphite, of roughly 25 mm in diameter and 32 mm long, into which a spherical fuel element (little pebble) of 20 mm in diameter, containing roughly 1650 particles, was incorporated (see Figure 2). The spherical fuel element is a little pebble, representative of a pebble which is the German HTR fuel reference element.

The data on the particles are gathered in the following table :

| Experiment | HFR-P4 1&3 Capsules | HFR-P4 2 Capsule |
|---|---|---|
| ***Kernel*** | | |
| Composition | $UO_2$ | $UO_2$ |
| O/M | 2.006 | 2.006 |
| Enrichment $^{235}U$ (%) | 9.82 | 9.82 |
| Diameter (µm) | 497 | 497 |
| Density (g/cm$^3$) | 10.8 | 10.8 |
| ***Layer thickness (µm)*** | (average values) | |
| Buffer | 94 | 93 |
| IpyC | 41 | 37 |
| SiC | 36 | 51 |
| OpyC | 40 | 38 |
| ***Layer density (g/cm$^3$)*** | (average values) | |
| Buffer | 1.00 | 1.00 |
| IpyC | 1.86 | 1.86 |
| SiC | 3.20 | 3.20 |
| OpyC | 1.88 | 1.87 |

The available irradiation data are :

| Capsule | 1 | 2 | 3 |
|---|---|---|---|
| Irradiation time (EFPD) | 351 | 351 | 351 |
| Peak burn-up (%FIMA) | 14.7 | 14.9 | 14.7 |
| Peak fluence($10^{25}$ n/m$^2$ E>16fJ) | 7.9 | 7.9 | 7.8 |
| Peak temperature (°C) | 940 | 945 | 1075 |

The values above are measured values. The temperature corresponds to the value given by a thermocouple located at the center of the compact, in the free fuel zone.

## 2.2. PHYSICAL AND MECHANICAL PROPERTIES OF MATERIALS

### 2.2.1. Kernel

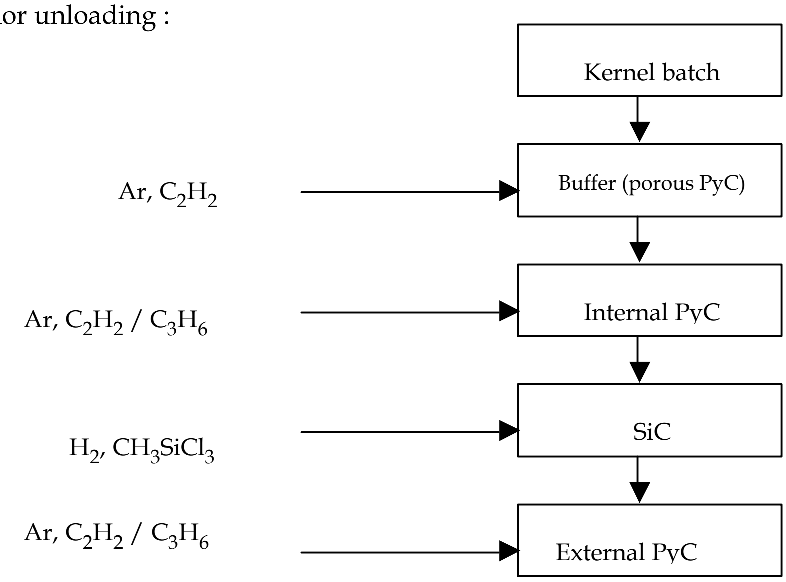
The kernels are made of low enriched $UO_2$ and were fabricated with the SOL-GEL process. The properties used for the modeling are those taken from Document *[3]* defined within the 5th FWP HTR-F project.

The properties used are density ρ, thermal conductivity λ (first law), coefficient of thermal expansion α, Young's modulus E and the Poisson ratio ν. The fuel creep (thermal and irradiation) is not taken into account at this stage.

The total porosity of the kernel is deduced from the theoretical density given in the note Ref. *[3]* and the fabrication density of the kernel (10.8) given in §2.1 : $p = (10.95 - \rho_{th})/10.95 = 0.0137$ (1.37%)

### 2.2.2. Layers

The layers were deposited by means of a CVD process according to the following sequence, without interruption nor unloading :



The properties which are used for the buffer, the PyC and SiC dense layers are thermal conductivity λ, the coefficient of thermal expansion α, the Young's modulus E, the Poisson's ratio ν and the irradiation creep law. Several calculation cases with different values for these properties were studied (see § 3.2). The values taken into account come from the note Ref *[3]* and are presented in Table 2. More particularly, the « BNFL » and « FZJ » data are those proposed by these organizations within the framework of the European HTR-F contract.

The simplified data are realistic but their evolution is simple and does not depend on either temperature nor fluence. The pyrocarbon irradiation induced dimensional change rate is constant (-2% for $10^{25}$ $n.m^{-2}$) and is the same in the three directions. The SiC irradiation creep is negligible. The objective of this set of data is to understand the phenomena and the influence of each parameter.

As an illustration and to set orders of magnitude, Figure 3 shows the evolution of Young's modulus for the Buffer and PyC layers in a representative operating range.

The porosity of the layers is deduced from the theoretical density of pyrocarbon and of SiC given in Ref *[3]* and from the layer density given in §2.1 :

| Layers | Theorical density ($g.cm^{-3}$) | Measured density ($g.cm^{-3}$) | Porosity (%) |
|---|---|---|---|
| Buffer | 2.26 | 1.00 | 55.8 |
| IPyC | 2.26 | 1.86 | 17.7 |
| SiC | 3.17 | 3.20 | 0.0 |
| OPyC | 2.26 | 1.88 | 16.8 |

## 2.3. LOADINGS

### 2.3.1. Thermal calculation

The thermal loading has two components :

- The power released by fission in the kernel. In the ATLAS application, this value is calculated using the number of fissions per second and per fuel volume unit, which is an input data, theoretically dependent on time. This last value is not provided in the note Ref. *[2]*. It is re-calculated using known data, namely burnup and irradiation time. This re-calculated value is thus an average value over the duration of the cycle. This last hypothesis is a simplifying one, in the absence of a simplified neutronic modulus which could take into account the depletion in $^{235}U$ and the enrichment in $^{239}Pu$ and other fissile isotopes. It is indeed to be noted that a fission rate of 14.7% for an initial enrichment of 9.82% in fissile isotopes necessarily implies an evolution from a predominant fission of $^{235}U$ atoms at the beginning of irradiation to a predominant fission of $^{239}Pu$ atoms created by capture in $^{238}U$ during irradiation. This hypothesis should however not have any significant influence on the result ; it is not however of a conservative nature since, if we assume that in reality the power decrease during irradiation, the actual load at the beginning of irradiation will be greater than the simulated load.

$TCF = 100.(\tau.t.M_{HM})/(N_a.\rho_{HM}.10^3)$ and $P = 10^6.E.e.\tau$ with :

| | | |
|---|---|---|
| TCF | burn-up fraction | (% FIMA) |
| $\tau$ | fission rate | (fissions.m$^{-3}$.s$^{-1}$) |
| t | time | (s) |
| $M_{HM}$ | molar atom weight | (g) |
| $N_a$ | Avogadro number | (6.0221.10$^{23}$) |
| $\rho_{HM}$ | heavy metal density | (kg.m$^{-3}$) |
| P | volumic power | (W.m$^{-3}$) |
| E | fission energy | (E=200 MeV) |
| e | conversion J/eV | (1.602.10$^{-19}$) |

| | |
|---|---|
| $\tau$ = 1.19.10$^{20}$ fissions.m$^{-3}$.s$^{-1}$ | $P_{particule}$ = 0.24 W |

for 14.7 %FIMA and 351 EFPD.

- The imposed temperature to the model. This is the temperature of the external surface of the external PyC layer. By simplification, this temperature is taken as equal to 1000°C.

### 2.3.2. Mechanical calculation

The loads of the mechanical calculations are of imposed pressure or deformation type and result from the following physical phenomena :

- *Release of fission gases Xe and Kr and production of CO* (formed with the buffer carbon and the oxygen released by fission of Uranium or Plutonium). These gases generate a pressure which is applied to the internal wall of the IPyC layer and on the external wall of the kernel. This pressure both depends on the volume of gas formed and on the free volume. The free volume as well as the volume of gas formed, then released, are calculation results (see §3.1).

The value chosen for the production of Xe and Kr is of 0.301 atom of gas formed for one split atom. Only part of the gas formed is released. The release model used is given in Ref. [3]. The CO production law is given in Ref. [3], §3.4.2, PROKSCH model. This law is valid for low enriched $UO_2$ fuels.

- *Influence of the graphite matrix of the compact on the particle*. This influence is, for the time being, taken into account by a pressure applied on the external OPyC layer. In a first stage, this pressure is taken as equal to 0.1 MPa.

- *Fuel swelling*. This includes the solid and gaseous swelling. The solid and gaseous swelling laws are given in Ref. [3]. These laws are expressed versus the mass burnup expressed in GWd/$t_{HM}$. In the ATLAS application, this last value is calculated at each time step using the number of fissions per second and per fuel volume unit, which is an input data. This value is not provided in the note Ref. [2]. It is calculated from known data, namely the final burnup and irradiation time (see §2.3.1).

- *Fuel densification*. The densification law is given in Ref. [3].

- *PyC and SiC layer irradiation induced dimensional change rate*. The laws are given in Ref. [3]. These laws are expressed versus the fast integrated flux. The flux not being provided in Ref. [2], it is taken as constant during the irradiation and as equal to the total fluence ($7.9.10^{25}$ $n.m^{-2}$) divided by the irradiation time, namely $\Phi = 2.6.10^{18}$ $n.m^{-2}.s^{-1}$. Figure 4 shows the evolution of the PyC and SiC deformation versus fluence.

### 2.4. CRITERIA TO BE RESPECTED

For the moment, there are no criteria to respect, the purpose of this document being to help in the definition of the most relevant design criteria.

## 3. CALCULATIONS

### 3.1. MODELING

A particle and eventually an additional layer around the particle to simulate the particle's environment are modeled. The modeling is detailed in Ref. [1]. It is briefly described below (see Figure 5).

A finite element method is used and is followed by :

- A thermal calculation giving the temperature field in the meshing nodes.

- A mechanical calculation allows access to the displacements fields, stresses and strains in the meshing nodes. The particle model is axisymmetrical, two-dimensional and represents a part of the particle.

The thermal model treats the conduction in the particle. Between the buffer and the kernel and between the buffer and the IPyC, meshes simulate a gaseous joint. The boundary conditions of this model are two-fold : a condition of nil flux on each side of the model and an imposed temperature on the particle external surface nodes. The conductivity of the layers and of the kernel is re-calculated at each time step and depends on the temperature, the integrated fluence and the fabrication and gaseous porosities. The porosity is re-calculated at each time step.

The mechanical model treats the visco-elasticity in the particle. The non-linearities are of two types : first, the material non-linearity through irradiation creep laws and second, the geometrical non-linearity through a contact condition between kernel and buffer and between buffer and IPyC. The layers are connected to each others. The main characteristics of the model are as follows :

- The thermal load is the temperature field resulting from the thermal calculation.

- The pressure load is calculated at each time step from the free volume (itself calculated from the deformed geometry), the temperature and the quantity of gas (Xe, Kr, CO) present. It is applied to the IPyC layer internal skin and to the kernel external skin.

The loads imposed by the swelling of the kernel and the irradiation induced deformation of the layers are considered as loads of imposed deformation type. These are taken into account by making an analogy between swelling and thermal expansion.

Table 1 gathers the input data. Table 2 summarizes the layer properties.

## 3.2. CALCULATIONS

The parametric calculations for the HTR particle in the HFR-P4 experiment were carried out to understand the behavior of the particle and measure the influence of some properties of PyC and SiC, more particularly :

-The irradiation induced creep coefficients of the dense pyrocarbon layers,

-The irradiation induced dimensional change of the dense pyrocarbon layers,

-The buffer characteristics.

That is why this evaluation grid was drawn up :

<table>
<tr><th rowspan="2">Calculated cases</th><th colspan="3">Properties</th><th rowspan="2">Comments</th></tr>
<tr><th>Buffer</th><th>PyC</th><th>SiC</th></tr>
<tr><td>Case 1</td><td>(1)</td><td colspan="2">Simplified</td><td>Reference case</td></tr>
<tr><td>Case 2</td><td>BNFL</td><td>BNFL</td><td>BNFL</td><td rowspan="2">Buffer stresses are prominent and not realistic because the buffer is not unbreakable. These calculations are not presented</td></tr>
<tr><td>Case 3</td><td>FZJ</td><td>FZJ</td><td>FZJ</td></tr>
<tr><td>Case 4</td><td rowspan="6">(1)<br>Thermal properties are taking into account but mechanical properties are specific : no irradiation induced dimensional change rate and very low Young modulus</td><td>BNFL</td><td>BNFL</td><td rowspan="5">These cases are discussed</td></tr>
<tr><td>Case 5</td><td>FZJ</td><td>FZJ</td></tr>
<tr><td>Case 124</td><td>Case 1 K/2</td><td>Case 1</td></tr>
<tr><td>Case 125</td><td>Case 1 K/5</td><td>Case 1</td></tr>
<tr><td>Case 126</td><td>Case 1 2K</td><td>Case 1</td></tr>
<tr><td>Case 13</td><td>Case 1</td><td>Case 1</td><td>(2)<br>Another layer has been added to take into account the compact environment. This calculation is not presented</td></tr>
</table>

K : creep coefficient

(1) : the buffer thermal characteristics are correctly represented. However, the mechanical characteristics are modified so that the buffer has no mechanical influence on the particle. Young's modulus is taken as very low (10 MPa) and the irradiation induced dimensional change is not taken into account. Actually, the buffer, by very rapidly irradiation induced dimensional change, failed, and no longer has any mechanical action on the external layers.

(2) : in the calculations other than those in case 13, the environment of the particle was not taken into account. In the case 13 calculation, to simulate the graphite surrounding the particle, a 4 mm layer was added with the properties of dense pyrocarbon and a irradiation induced dimensional change rate of 1% for $10^{26}$ n.m$^{-2}$, in other terms, twenty times less than those of the reference pyrocarbon. The influence of

this layer does not raise any questions on the analysis of the results from other calculations but should be carefully analyzed during the next studies.

## 3.3. RESULT ANALYSIS

### 3.3.1. Reference calculation

The calculation results are shown in table 3 and Figures 7 to 11.

*Thermal calculation*

Figure 7 shows the evolution of temperature in the kernel and in the layers versus fluence as well as a cross section of the temperature in the particle at the end of irradiation.

The ΔT in the kernel is worth 12.7°C at the beginning of irradiation and 21.0°C at the end of irradiation. These values are those expected (analytically $\Delta T = P_{vol}.R^2/6\lambda$). The increase in the temperature gradient is due to the deterioration of the thermal conductivity of $UO_2$ with irradiation.

The ΔT in the gaseous gap between the buffer and the IPyC increases with irradiation and reaches at the end of irradiation 73.4°C. Indeed, the gas conductivity deteriorates and the gap increases, going from 0.2 µm (initial gap, arbitrarily set and creating a temperature delta less than the degree) to 11.2 µm.

The irradiation induced dimensional change of PyC is considered, for this first approach, as isotropic and is taken as equal to the tangential densification *[3]* in the three directions (whereas in reality the circumferential densification is accompanied, when there is a significant fluence, by a slight radial swelling, see BNFL and FZJ data, figure 4). Our hypothesis raises the radial displacement and therefore the gap. Thus, the calculated value of ΔT in the gap is likely not very realistic. This analysis is confirmed by calculations with BNFL and FZJ data sets.

*Mechanical calculation*

The irradiation induced dimensional change of the pyrocarbon layers (-2% by $10^{25}$ $n.m^{-2}$) is countered by the SiC layer, which is about 10 times more rigid. Figure 9 shows that the SiC layer is only displaced by its own expansion. This pyrocarbon dimensional change quickly creates circumferential compression stresses in the SiC layer and tensile stresses in the pyrocarbon layers. The irradiation induced creep in the pyrocarbon layers tends to relax the stresses before the latter become too great and an equilibrium is created between densification and relaxation. This equilibrium is reached very early on during irradiation (~$0.5.10^{25}$ $n.m^{-2}$, in other words, in the case of the HFR-P4 irradiation, after roughly twenty EFPD). The circumferential stress reaches an equilibrium at –163.2 MPa in the SiC layer and at 95.4 MPa in the IPyC layer (see Figure 8). This behavior is in agreement with the particle calculations presented in *[4]*.

Once this equilibrium is reached, the pressure in the particle free volume due to the release of fission gases and of the CO increases and changes the stress on the layers : the compression stress in the SiC layer starts decreasing (in absolute value) until -31.4 Mpa.

Thus, it would seem that the « reasonable » stress level reached in the PyC and SiC layers is obtained thanks to the irradiation induced creep of PyC. The creep deformation of the PyC layers is therefore very high, since it largely exceeds 10%. However, we do not know whether such an amplitude in deformation could lead to failure or not.

Beyond $3.10^{25}$ $n.m^{-2}$, the evolution of the pressure in the particle is nearly linear : at the end of irradiation it reaches 134.7 bars. This pressure depends mainly on the production and release of fission gases. The CO production, with the PROKSCH model is very low (see Figure 10). The free volume, in our model, increases during the entire irradiation time because of the densification of the IPyC layer (see Figure 10). Because the densification is over-estimated, this pressure value is likely under-estimated.

### 3.3.2. PyC creep constant influence

The calculation cases 124, 125 and 126 were made so as to quantify the irradiation induced creep coefficient of the PyC layers, which were respectively divided by 2, divided by 5, and multiplied by 2. The results are shown in Table 4 and Figure 14.

<u>For a given irradiation induced dimensional change rate (independent from creep), the stress is strictly inversely proportional to the irradiation induced creep coefficient.</u>

The value of the creep coefficient in Case 125 (reference value divided by 5), which is not very far from the value proposed by FZJ, leads to high tensile stresses (~500 MPa) in the pyrocarbon at the beginning of irradiation. Hence, the SiC layer is never put under tension, except in the first instants under the effect of the thermal load. Nevertheless, such a high PyC tensile stress could lead to PyC rupture and modify the stress field in the SiC layer.

On the opposite, a high creep coefficient (Case 126, reference value multiplied by 2), which is favorable to the stress level in the pyrocarbon layers, can be unfavorable at the end of irradiation for the SiC layer.

### 3.3.3. Calculations with the laws proposed by FZJ

The differences between the calculation with the FZJ laws and the reference case are :

- The irradiation induced dimensional change of the pyrocarbon layers is described in the two directions (radial and tangential, see figure 4).
- The irradiation induced dimensional change of the pyrocarbon layers is lower,
- The irradiation induced creep coefficient of the pyrocarbon is 4 times less (to be compared to Case 125),

The irradiation creep coefficient of the SiC layer is more than 150 times greater than the creep coefficient of the pyrocarbon layers : this is similar to the reference case.

The results of the thermal calculation are shown in Table 4 and Figure 18. The evolution over time of temperature is rather different to that of the reference case. The maximum temperature is of 1064.5 °C in the kernel and occurs when the gap size is maximum. These temperatures are less than those in the reference case. The internal pyrocarbon layer begins to shrink in the radial direction, opening the gap like in the reference case, but, after $3.10^{25}$ $n.m^{-2}$, it swells and closes the gap again, decreasing the temperature.

The results of the mechanical calculation are shown in Table 4 and Figures 19 and 20. The level of the stresses at equilibrium is very high : 395.0 Mpa in the IPyC layer and –702.3 MPa in the SiC layer. Compared to the reference case, the stress ratio nearly corresponds to the irradiation induced creep coefficients ratio ($\sigma_{FZJ}/\sigma_{REF} \sim K_{REF}/ K_{FZJ}$). This is logical if and only if the irradiation induced deformation rates under fast flux are identical since, according to ***[4]***, the stress ratio at equilibrium must be as follows :

$$\sigma_{REF} = Cste*(g'_{REF}/K_{REF}) \text{ and } \sigma_{FZJ} = Cste*(g'_{FZJ}/K_{FZJ})$$

$$\text{from which} \quad \sigma_{FZJ}/\sigma_{REF} = (K_{REF}/ K_{FZJ})*(g'_{FZJ}/ g'_{REF})$$

It would seem that initially, according to Figure 4, the irradiation induced dimensional change rate under fast flux proposed by FZJ is lower than that of the reference case. One could thus expect a lower stress level than the one found :

$$\text{If } g'_{FZJ}/ g'_{REF} < 1 \text{ then } \sigma_{FZJ}/\sigma_{REF} < K_{REF}/ K_{FZJ}$$

Actually, the level is higher than that expected because, at the very beginning of irradiation, the deformation rates are nearly equivalent ($g'_{FZJ} \sim g'_{REF}$ , see Figure 4). And it is at this irradiation time that the equilibrium is reached.

This calculation evidences the importance of knowing the deformation rate under fast flux at the beginning of irradiation. In our case, it would seem likely that the deformation rate at low fluence is not very accurate since it comes from an adjustment with the data corresponding to greater fluences.

### 3.3.4. Calculations with the laws proposed by BNFL

The differences between the calculation with the BNFL laws and the reference case are :

- The irradiation induced dimensional change of the pyrocarbon layers is described in the two directions (radial and tangential, see figure 4). We can note that the radial shrinkage is more important than for FZJ.

- The irradiation induced creep coefficient of the pyrocarbon is 1.3 times less.

The results of the thermal calculation are shown in Table 4 and Figure 15. The evolution over time of temperature is rather different to that of the reference case. The maximum temperature is of 1064.3 °C in the kernel and occurs when the gap size is maximum. These temperatures are less than those in the reference case. The internal pyrocarbon layer begins to shrink in the radial direction, opening the gap like in the reference case, but, after $4.10^{25}$ $n.m^{-2}$, it swells and closes the gap again, decreasing the temperature.

The results of the mechanical calculation are shown in Table 4 and Figures 16 and 17. The level of the stresses at equilibrium is 182.6 Mpa in the IPyC layer and –274.7 MPa in the SiC layer.

At the end of the irradiation, it seems to be that the irradiation induced dimensional change rate increase slightly, likely due to the fitting, but it is enough to stop the SiC stress increase due to the pressure increase. This phenomena has to be investigated more deeply because it is likely not realistic.

# 4. CONCLUSIONS

This document presents the first deterministic thermal and mechanical calculations on a free particle using the ATLAS.V1.0 European code. These calculations were based on the HFR-P4 experimental irradiation of little pebbles in the HFR reactor.

The behavior laws and material characteristics were gathered within a European framework. Concerning the PyC and SiC layers, and in addition to a simplified reference set, two property sets were used : one from the English BNFL company and one from the German research organization FZJ.

The thermal and mechanical behavior of the particle under irradiation is a complex phenomenon with many parameters. The different property sets led to rather different results, from both a thermal and mechanical point of view.

This first approach helped identify the following important parameters :

- The deformation kinetics under fast flux of the pyrocarbon layers and particularly at the beginning of irradiation,

- The irradiation induced creep coefficient of the PyC layers, but also that of the SiC layer,

- The failure modes of the layers.

- The behavior of the buffer. Here it would be useful to know its structural evolution as well as its thermal conductivity under fast flux.

This improved knowledge on these properties of PyC and SiC layers is an important step for the design basis and understanding of the in pile behavior of future fabrications. It entails the fine re-interpretation of past experiments and the achievement of analytical irradiation experiments on materials elaborated under the same conditions as those for future fabrications.

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# LIST OF TABLES

TABLE 1 : GENERAL DATA

| **Kernel** | Material | Enrichment | Diameter | Porosity | Stœchiometry |
|---|---|---|---|---|---|
| | $UO_2$ | 9.82 % | 497 µm | 1.37 % | 2.008 |

| **Layers** | Material | thickness | Porosity |
|---|---|---|---|
| 1st layer (Buffer) | porous pyrocarbon | 94 µm | 55.75 |
| 2nd layer | dense pyrocarbon | 41 µm | 17.70 |
| 3rd layer | SiC | 36 µm | 0.00 |
| 4th layer | dense pyrocarbon | 40 µm | 16.81 |
| Irradiation time | 351 EFPD | | |
| Flux | $2.6.10^{18}$ $n.m^{-2}.s^{-1}$ (*) | | |
| Fission rate | $1.19.10^{20}$ $fissions.m^{-3}.s^{-1}$ (*) | | |
| Temperature | 1000°C | | |
| External pressure | 0.1 MPa | | |
| Pressure (BOL) | 0.1 MPa | | |

(*) average values from total burn up and fluence.

TABLE 2 : LAYER PROPERTIES

| Parameter | Simplified data | BNFL data | FZJ data |
|---|---|---|---|
| **PyC layers (IPyC et OPyC)** | | | |
| λ ($W\ m^{-1}\ K^{-1}$) | 4 | See *[3]* | 4 |
| α ($10^{-6}\ K^{-1}$) | 5.5 | 5.6 | 5.5 |
| E (MPa) | $30\ 10^{9}$ | See *[3]* and figure 3 | $29\ 10^{3}$ |
| ν (/) | 0.3 | 0.21 | 0.3 |
| K ($MPa\ n\ m^{-2}$) | $5.8\ 10^{-29}$ | $4.4\ 10^{-29}$ | $1.4\ 10^{-29}$ |
| Irradiation induced dimensional change | -0.02*Φt | See *[3]* and figure 4 | See *[3]* and figure 4 |
| **SiC layer** | | | |
| λ ($W\ m^{-1}\ K^{-1}$) | 20 | 8.24 | 16 |
| α ($10^{-6}\ K^{-1}$) | 5 | 5 | 5 |
| E (MPa) | $429\ 10^{9}$ | $421.10^{3}$ | See *[3]* |
| ν (/) | 0.3 | 0.33 | 0.3 |
| K ($MPa\ n\ m^{-2}$) | $3.8\ 10^{-38}$ | $1.68\ 10^{-31}$ | $8.4\ 10^{-32}$ |
| Irradiation induced dimensional change | 0 | $6.6\ 10^{-4}$*Φt | See *[3]* |
| **Buffer** | | | |
| λ ($W\ m^{-1}\ K^{-1}$) | 0.5 | 0.5 | See *[3]* |
| α ($10^{-6}\ K^{-1}$) | 3.5 | 3.5 | 3.5 |
| E (MPa) | $1\ 10^{7}$ | See *[3]* | See *[3]* |
| ν (/) | 0.3 | 0.21 | 0.3 |
| K ($MPa\ n\ m^{-2}$) | $3.8\ 10^{-28}$ | $4.4\ 10^{-29}$ | $9.6\ 10^{-30}$ |
| Irradiation induced dimensional change | 0 | See *[3]* | See *[3]* |

TABLE 3 : : REFERENCE CASE MAIN RESULTS

| | 0 EFPD | 1 EFPD | 20 EFPD | 180 EFPD | 351 EFPD |
|---|---|---|---|---|---|
| Burn up (%FIMA) | 0 | 0.04 | 0.83 | 7.66 | 15.00 |
| Burn up (MW/j/t) | 0 | 377 | 7 799 | 71 947 | 138 101 |
| Fluence ($10^{25}$ n $m^{-2}$) | 0 | 0.02 | 0.45 | 4.12 | 7.90 |
| Kernel swelling (%) | 0 | 0.02 | 0.33 | 1.75 | 3.14 |
| Radial displacement (µm) | 0.2 | 0.2 | 0.4 | 6.7 | 11.2 |
| Gap conductivity ($W.m^{-1}.K^{-1}$) | 0.01 | 0.02 | 0.021 | 0.022 | 0.024 |
| Tmax kernel (°C) | 20 | 1061.0 | 1062.5 | 1108.9 | 1137.2 |
| ΔT kernel (°C) | 0 | 12.7 | 13.0 | 17.1 | 21.0 |
| ΔT joint (°C) | 0 | 1.6 | 2.6 | 47.0 | 73.4 |
| IPyC radial and tangential strain (%) | 0.0 | 0.0 | -0.9 | -8.2 | -15.8 |
| Pressure (bars) | 1.0 | 4.4 | 4.9 | 54.2 | 134.7 |
| SiC tangential stresses (MPa) | 0.0 | 3.3 | -163.2 | -102.5 | -31.4 |
| IPyC tangential stresses (MPa) | 0.0 | -1.4 | 95.4 | 86.9 | 73.7 |
| OPyC tangential stresses (MPa) | 0.0 | -0.4 | 58.2 | 61.2 | 63.0 |

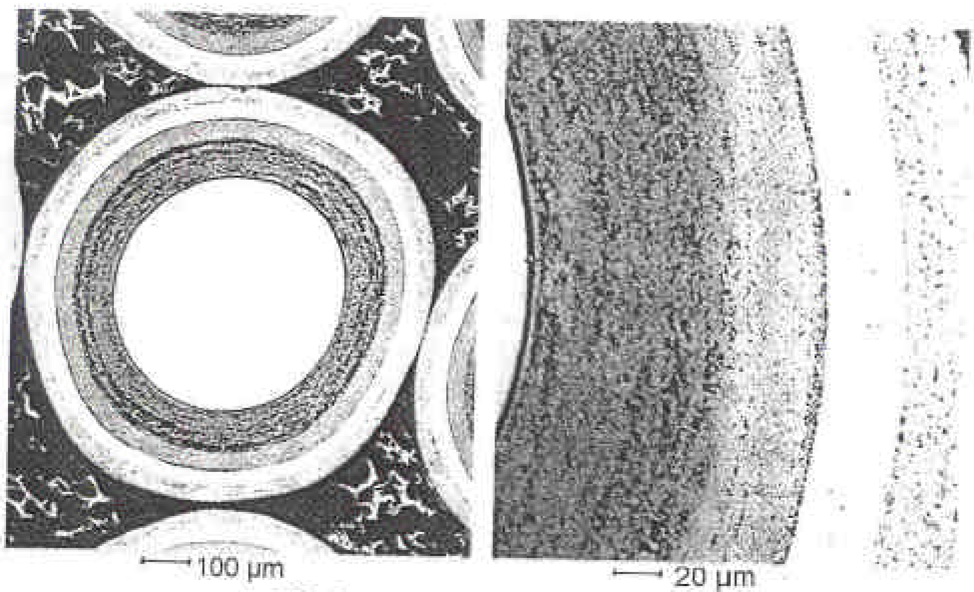
## TABLE 4 : RESULT COMPARISON

| | Référence cas 1 | BNFL cas 4 | FZJ cas 5 |
|---|---|---|---|
| Gap (µm) | 11.2 | 0.2 | 0.2 |
| Tmax kernel (°C) | 1137.2 | 1064.3 | 1064.5 |
| ΔT kernel (°C) | 21.0 | 20.5 | 20.4 |
| ΔT gap (°C) | 73.4 | 1.5 | 1.5 |
| Radial strain IPyC (%) | -15.8 | 32.0 | 16.8 |
| Tangential strain IPyC (%) | -15.8 | -16.1 | -9.6 |
| Pressure (bars) | 134.7 | 171.1 | 174.7 |
| SiC maximum tangential stress(MPa) | 37.5 | 32.1 | 26.6 |
| SiC minimum tangential stress (MPa) | -163.6 | -274.7 | -702.3 |
| IPyC maximum tangential stress (MPa) | 96.6 | 182.6 | 395.0 |
| IPyC minimum tangential stress (MPa) | -18.7 | -14.6 | -13.2 |

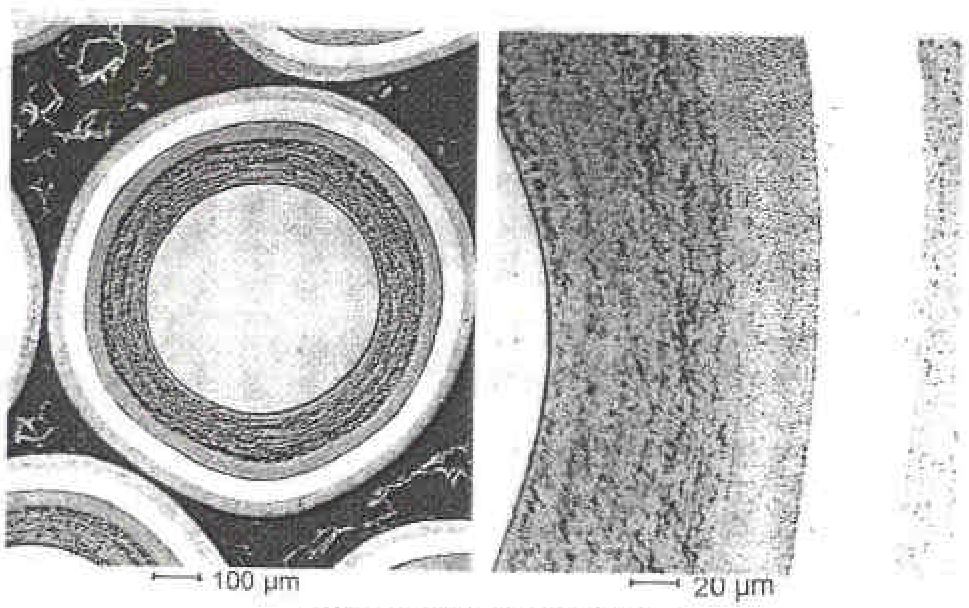
| | K/2 cas 124 | K/5 cas 125 | 2K cas 126 |
|---|---|---|---|
| Gap (µm) | 11.1 | 10.8 | 11.3 |
| Tmax kernel | 1136.0 | 1134.7 | 1137.9 |
| ΔT kernel | 21.0 | 21.0 | 21.1 |
| ΔT gap (K) | 72.8 | 70.9 | 74.0 |
| IPyC radial and tangential strain (%) | -15.8 | -15.8 | -15.8 |
| Pressure (MPa) | 134.9 | 135.4 | 134.4 |
| SiC maximum tangential stress(MPa) | 37.8 | 38.0 | 36.8 |
| SiC minimum tangential stress (MPa) | -320.9 | -761.0 | -81.4 |
| IPyC maximum tangential stress (MPa) | 192.4 | 477.0 | 48.3 |
| IPyC minimum tangential stress (MPa) | -18.9 | -19.0 | -18.5 |

## LIST OF FIGURES

## FIGURE 1 : HFR-P4 PARTICLE CROSS SECTION




**SiC layer thickness 36 µm**




**SiC layer thickness 51 µm**

FIGURE 2 : HFR-P4 X-RADIOGRAPHY

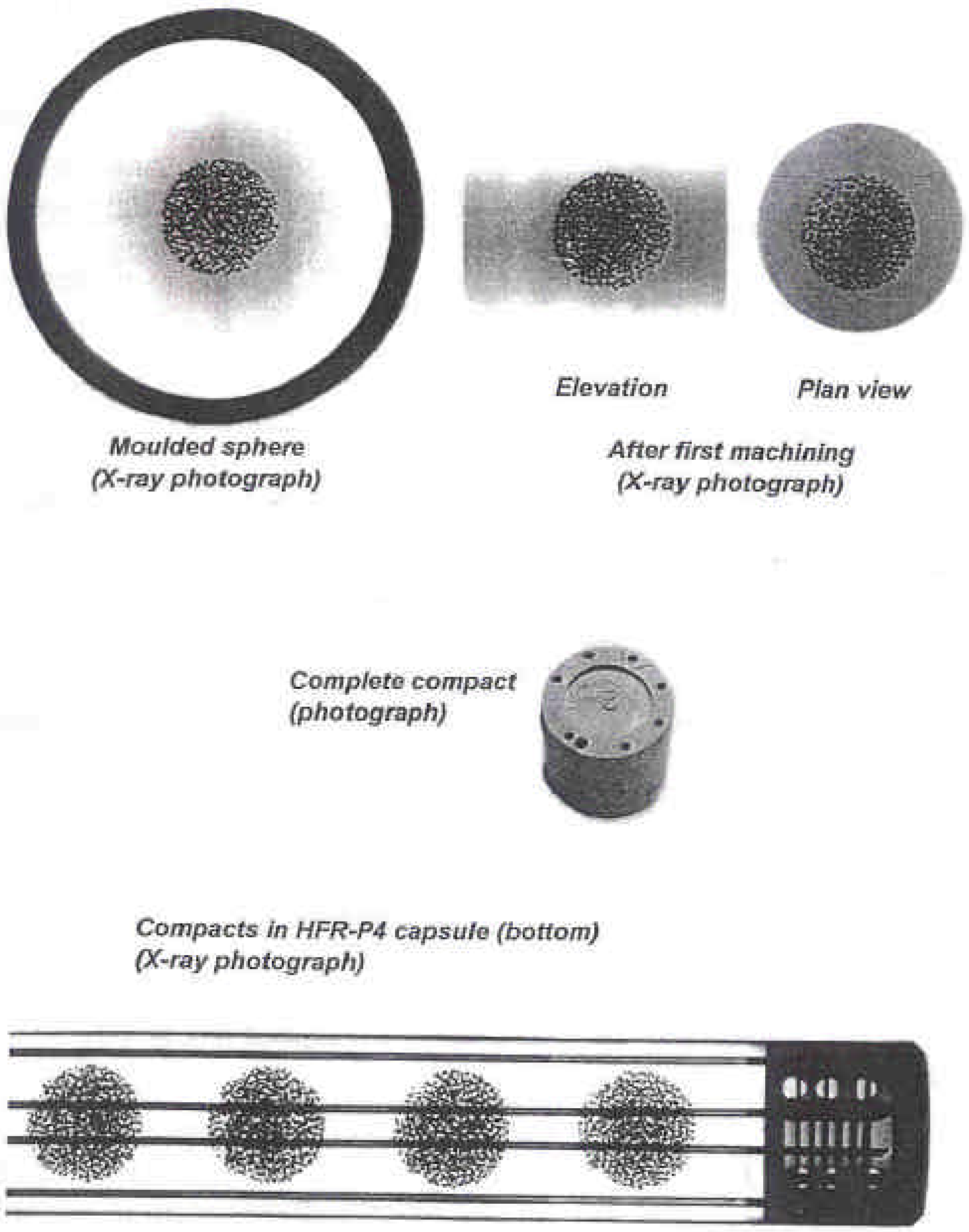


FIGURE 3 : YOUNG MODULUS

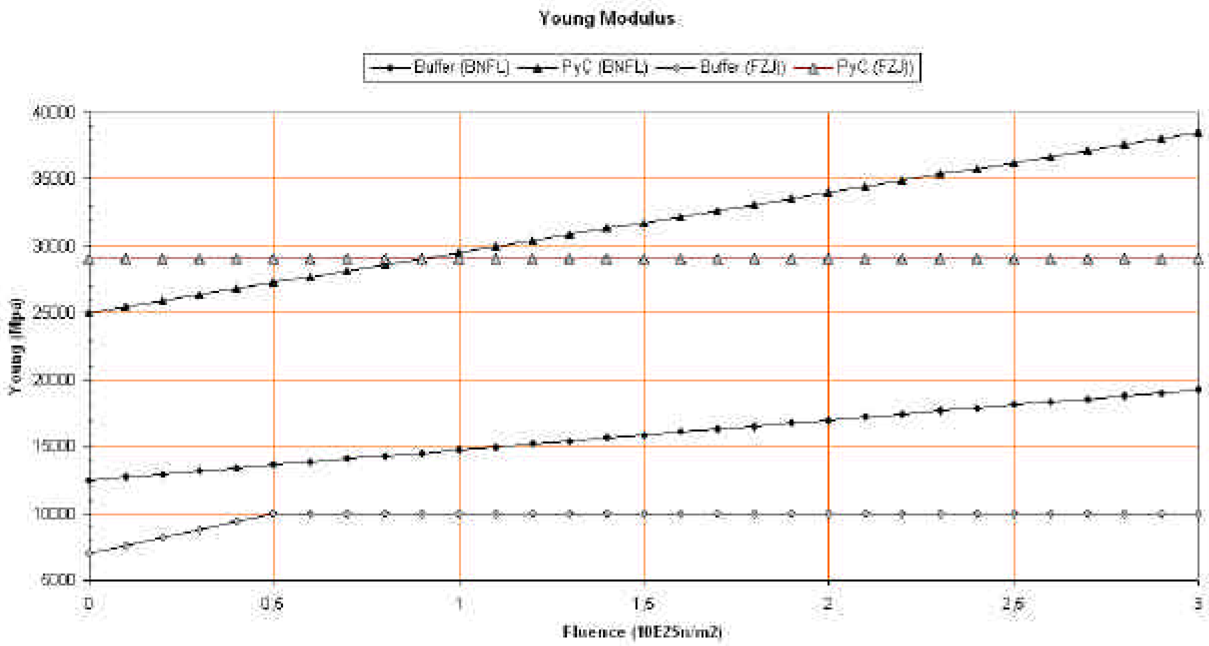
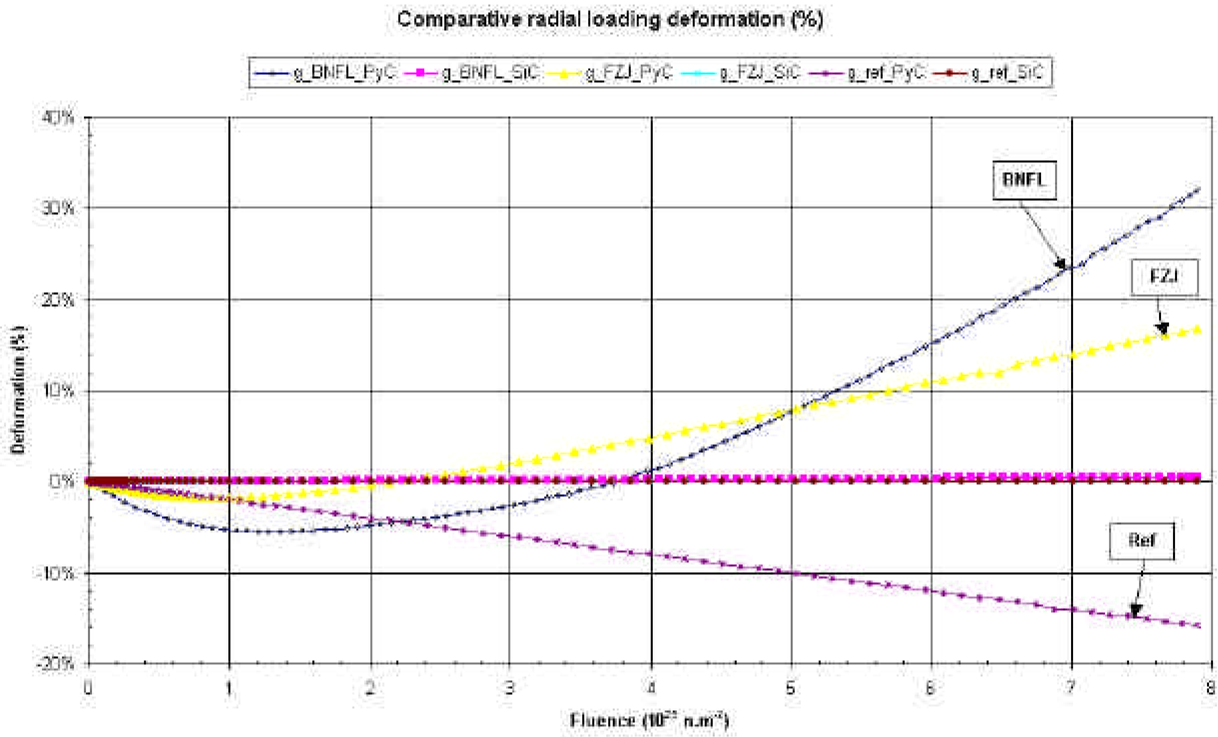


FIGURE 4 : PYC AND SIC IRRADIATION INDUCED DEFORMATION



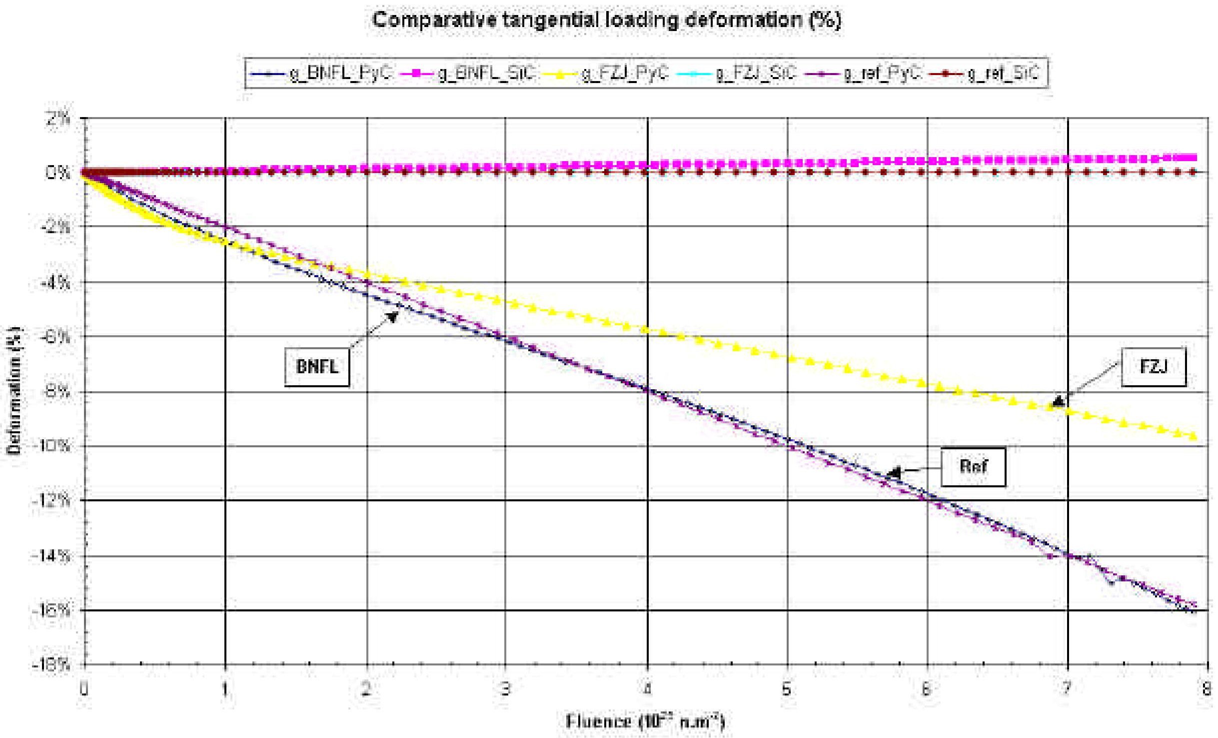



FIGURE 5 : MESH

Mecanical and thermal meshing model.

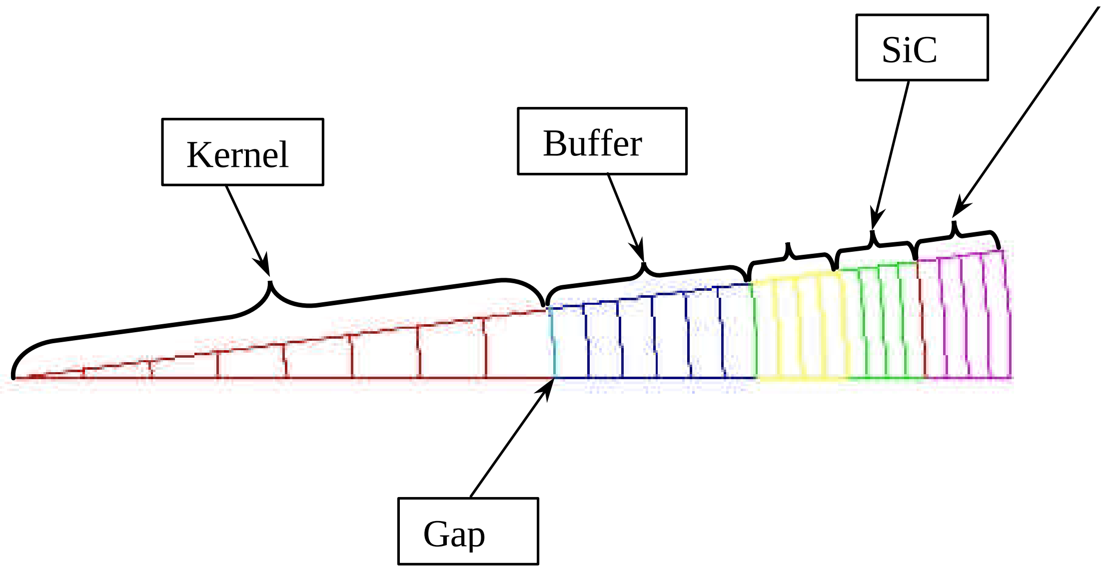
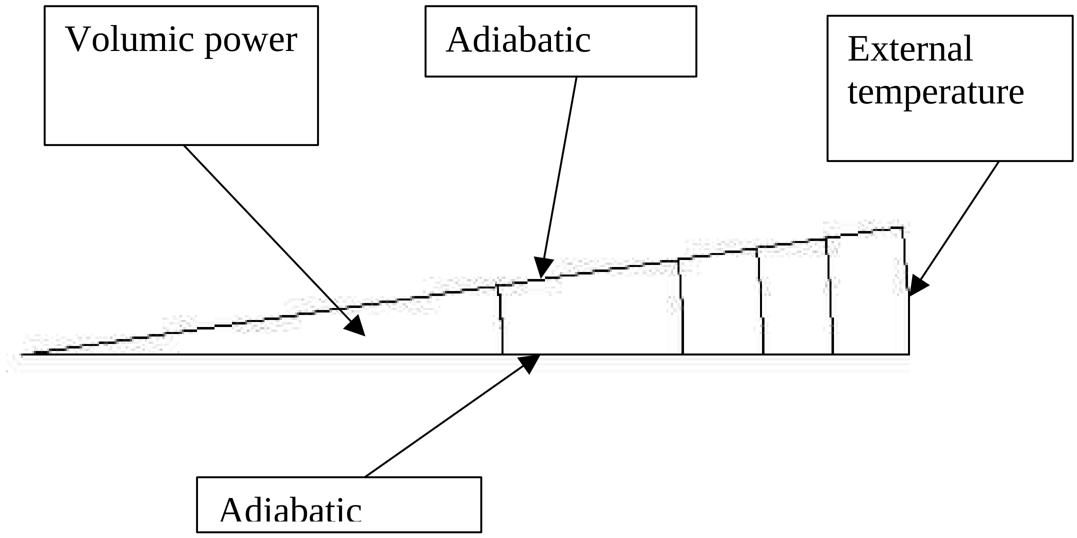


FIGURE 6 : LOADINGS AND BOUNDARY CONDITIONS

Loadings and boundary conditions of the thermal model.




Loadings and boundary conditions of the mechanical model

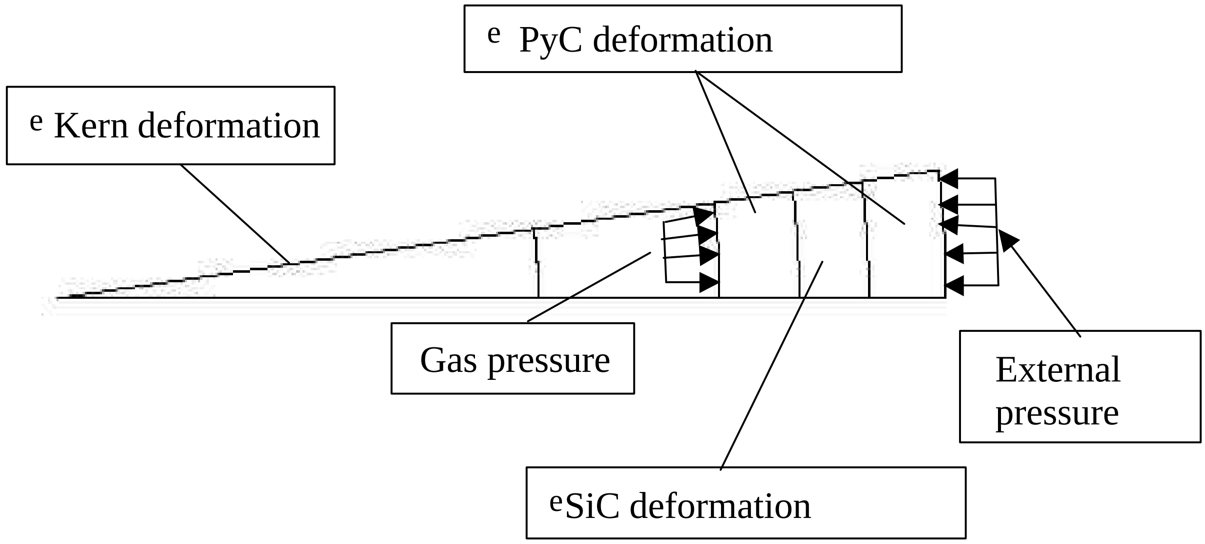
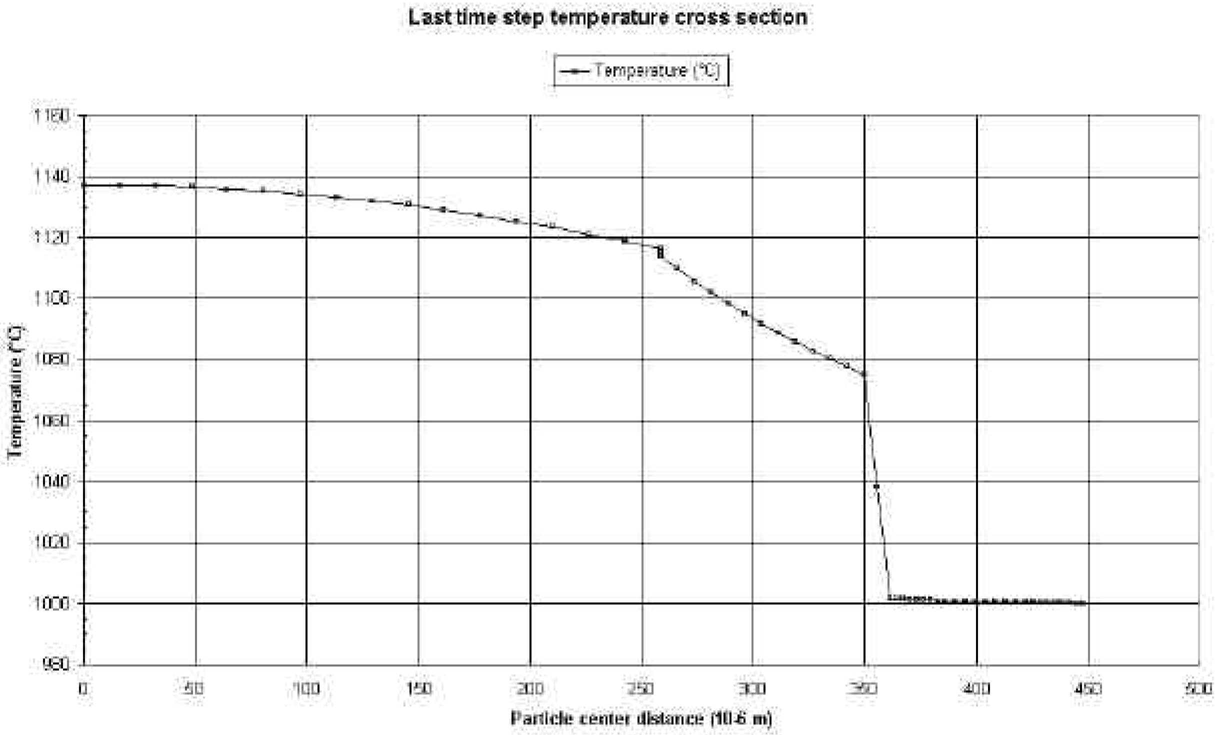
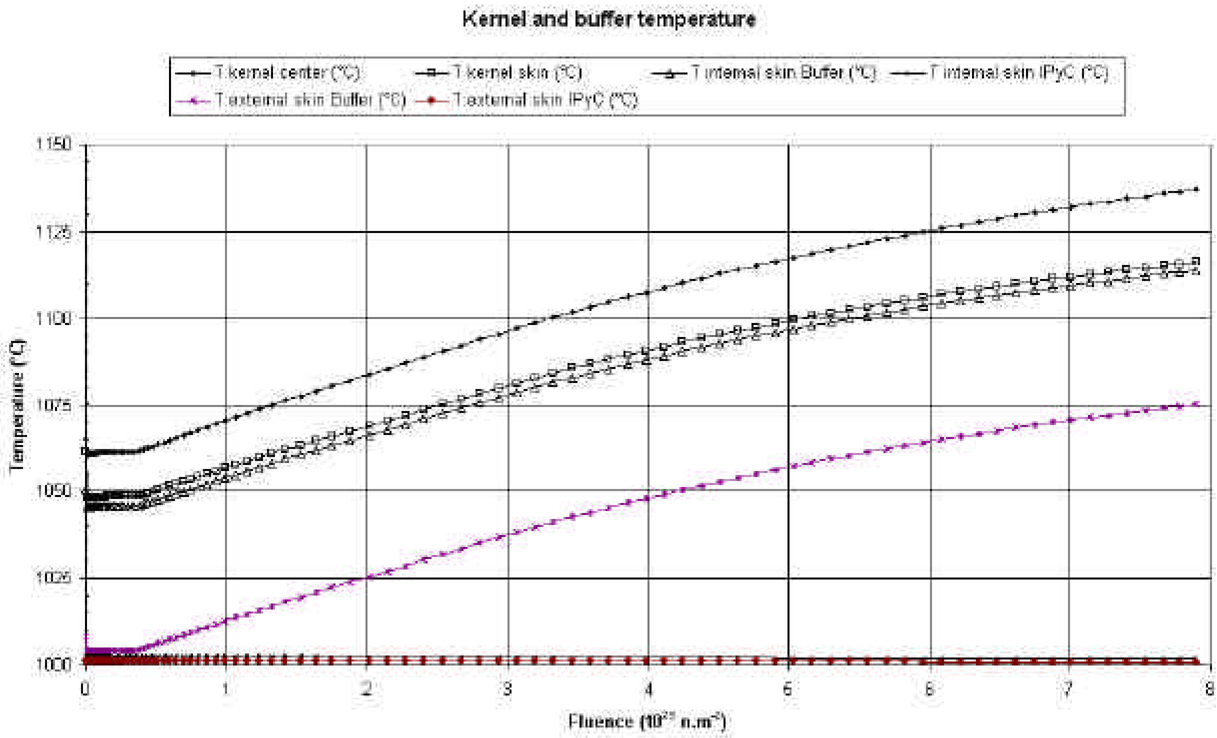
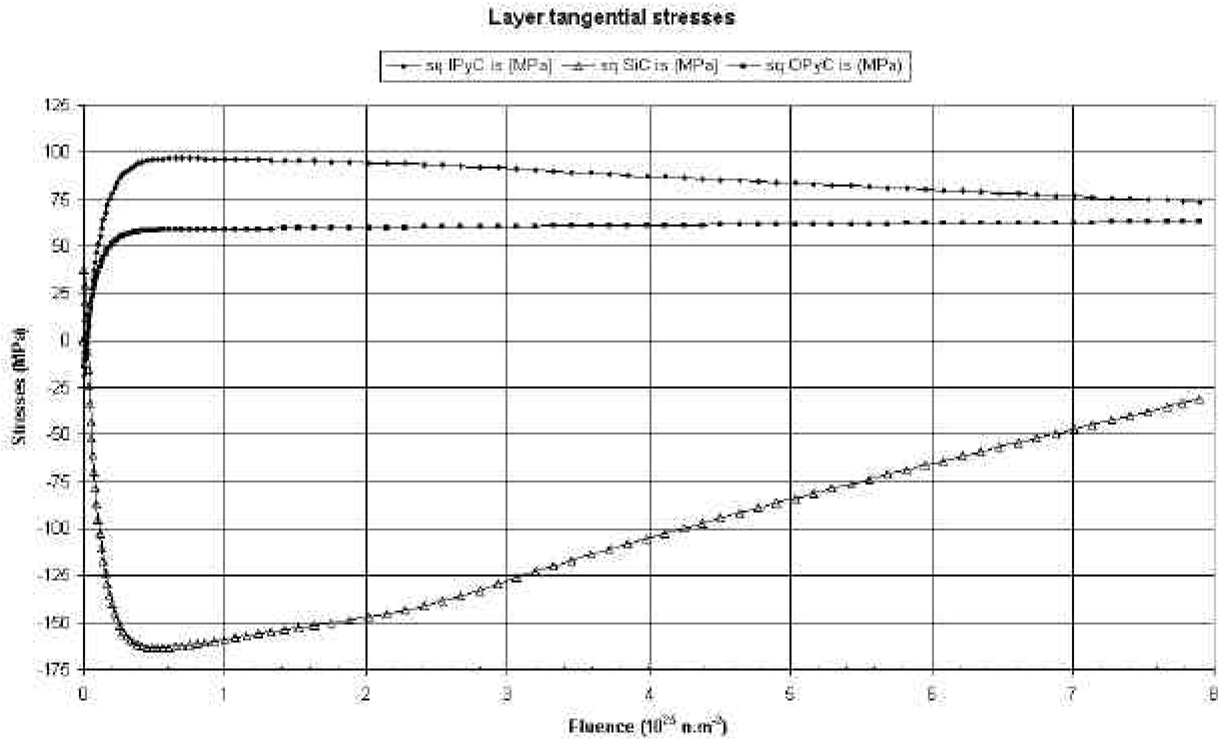


FIGURE 7 : REFERENCE CALCULATION – THERMAL RESULTS



## FIGURE 8 : REFERENCE CALCULATION – LAYER STRESSES



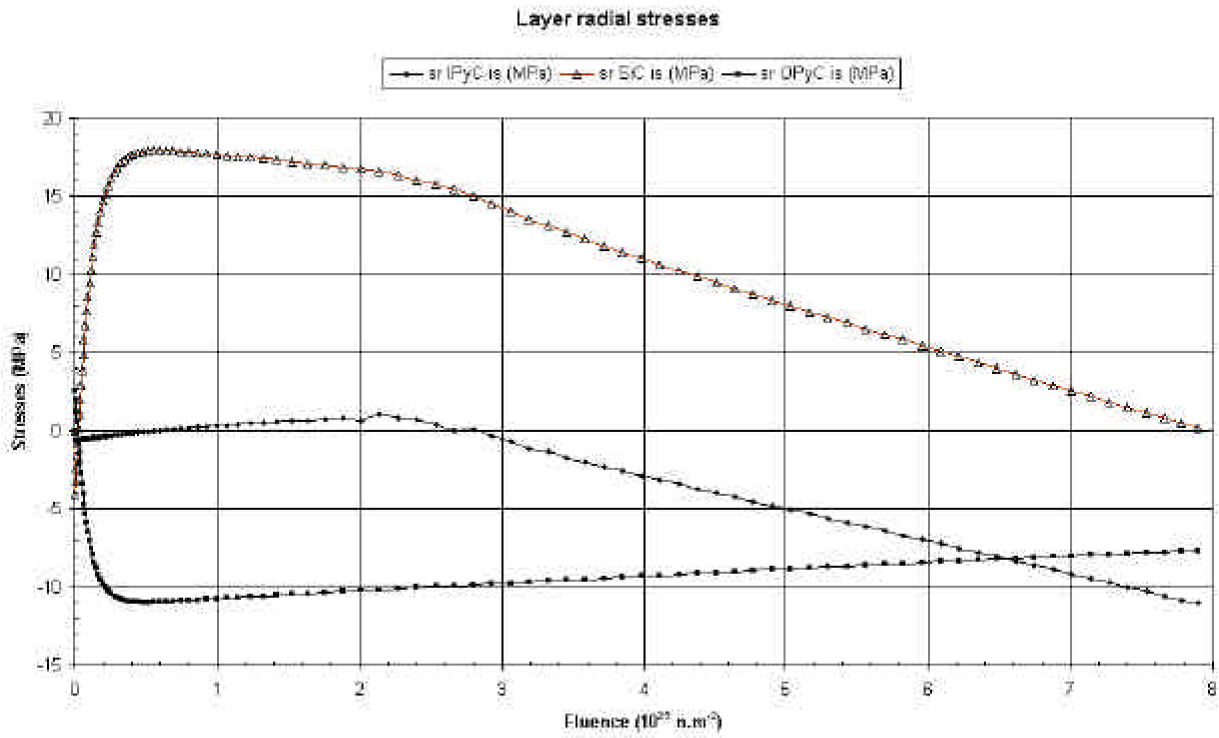
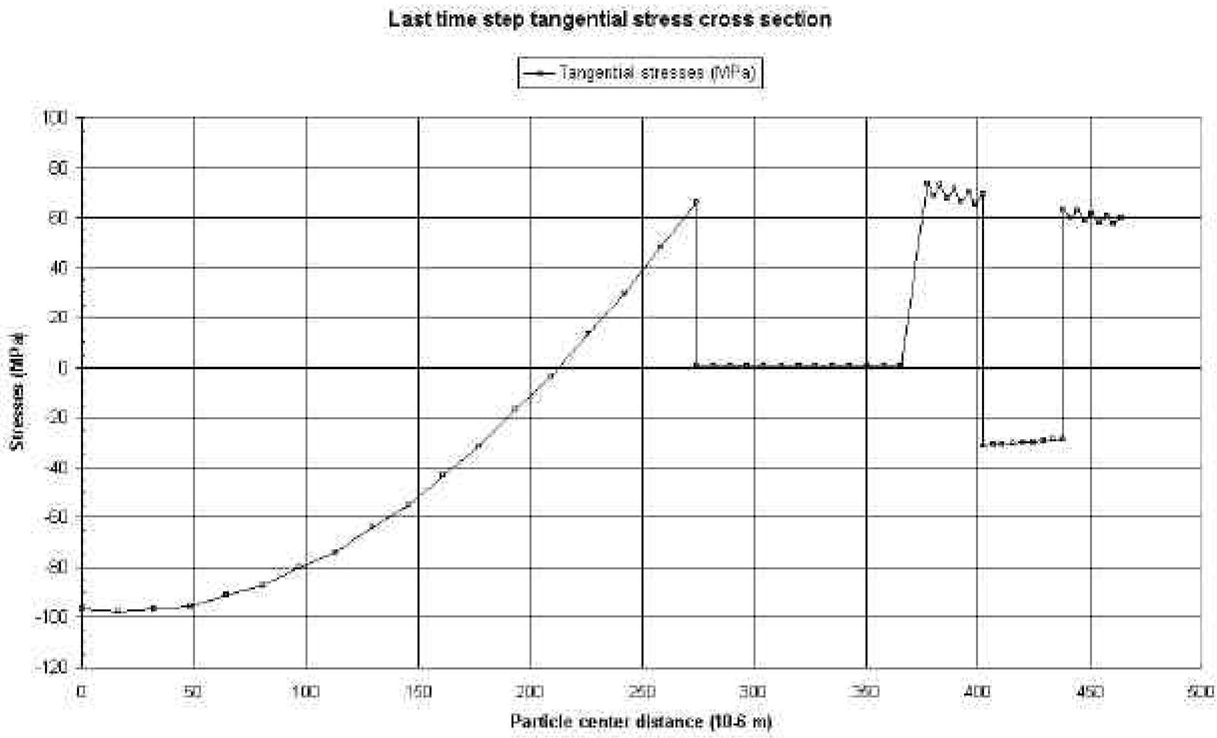
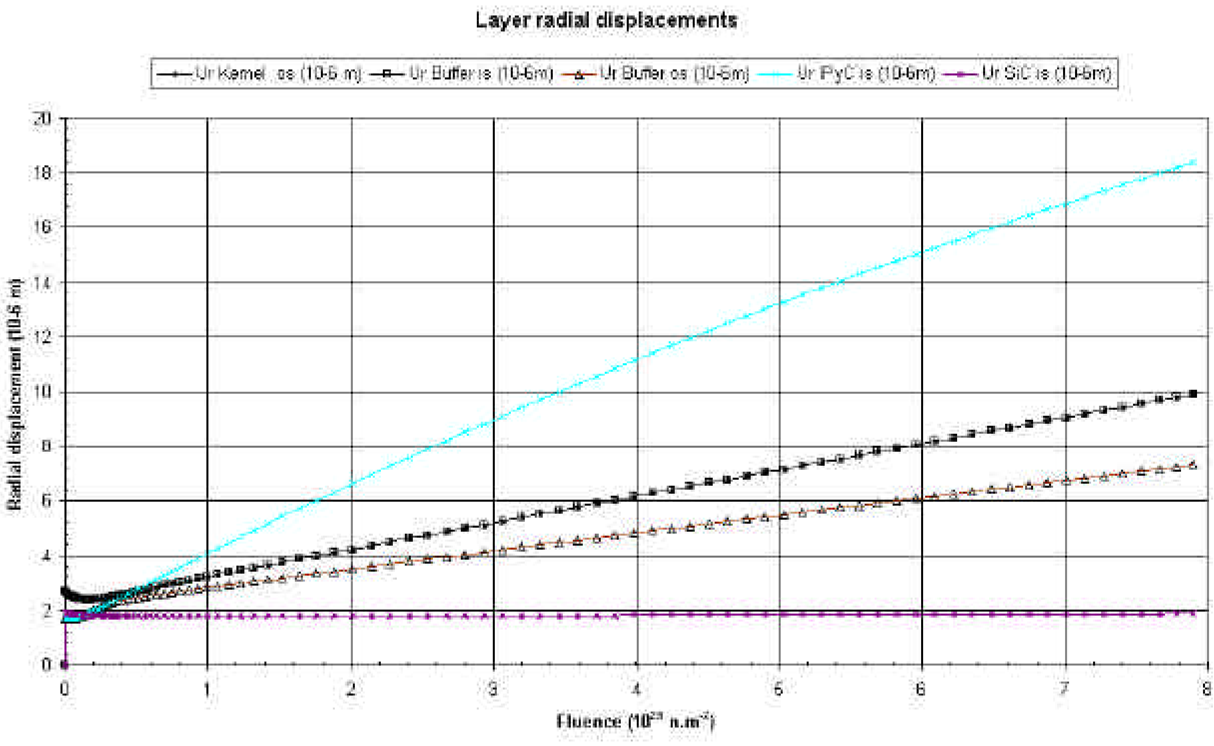
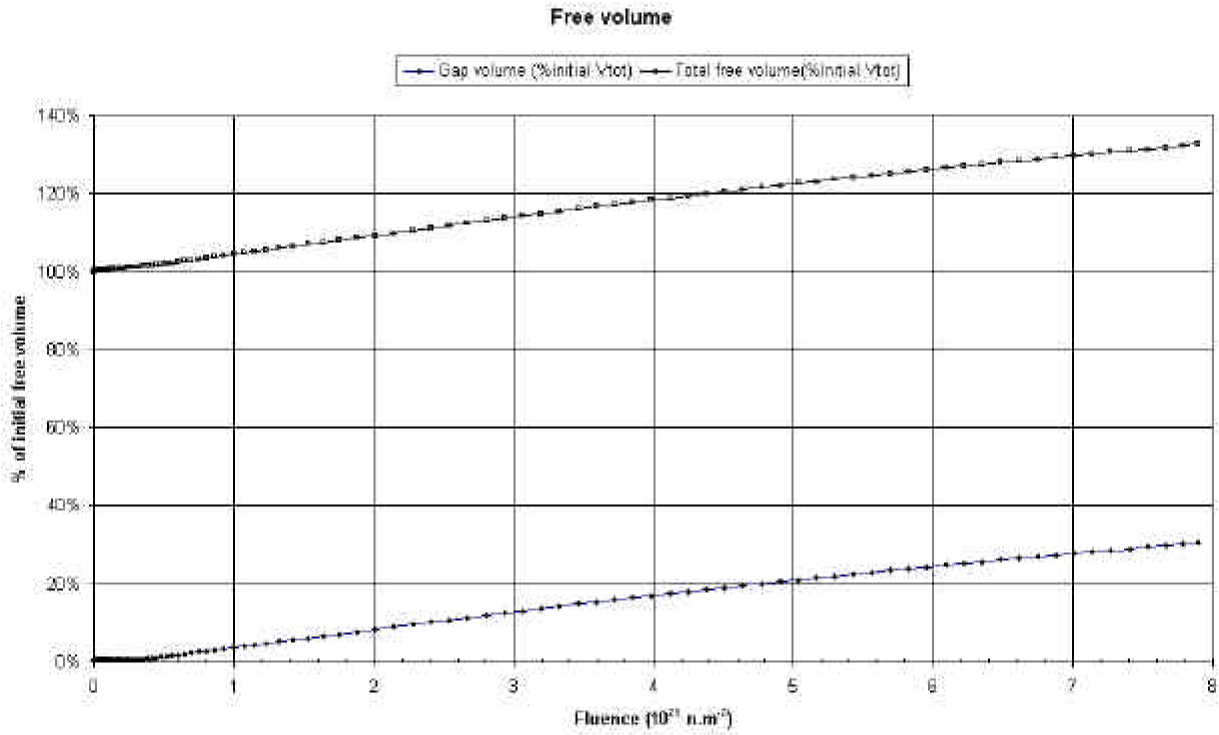



FIGURE 9 : REFERENCE CALCULATION – LAYER STRESS AND STRAIN



IGURE 10 : REFERENCE CALCULATION – FREE VOLUME AND GAS PRODUCTION



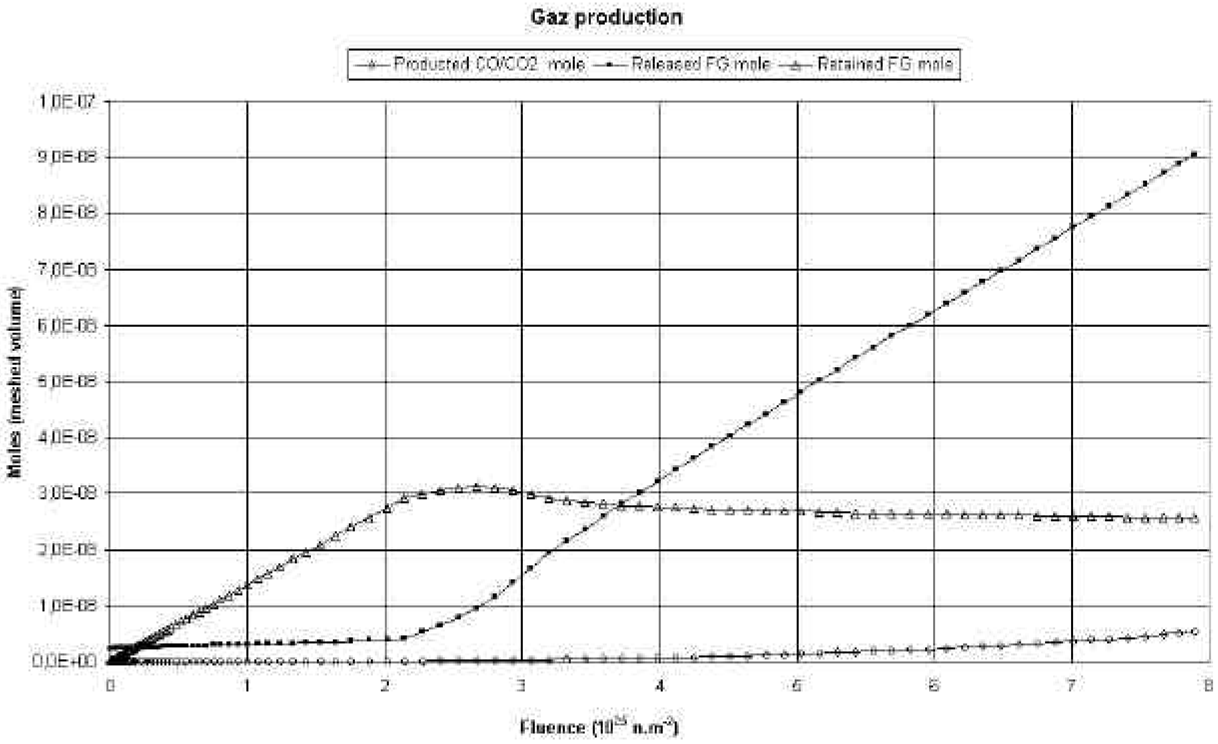
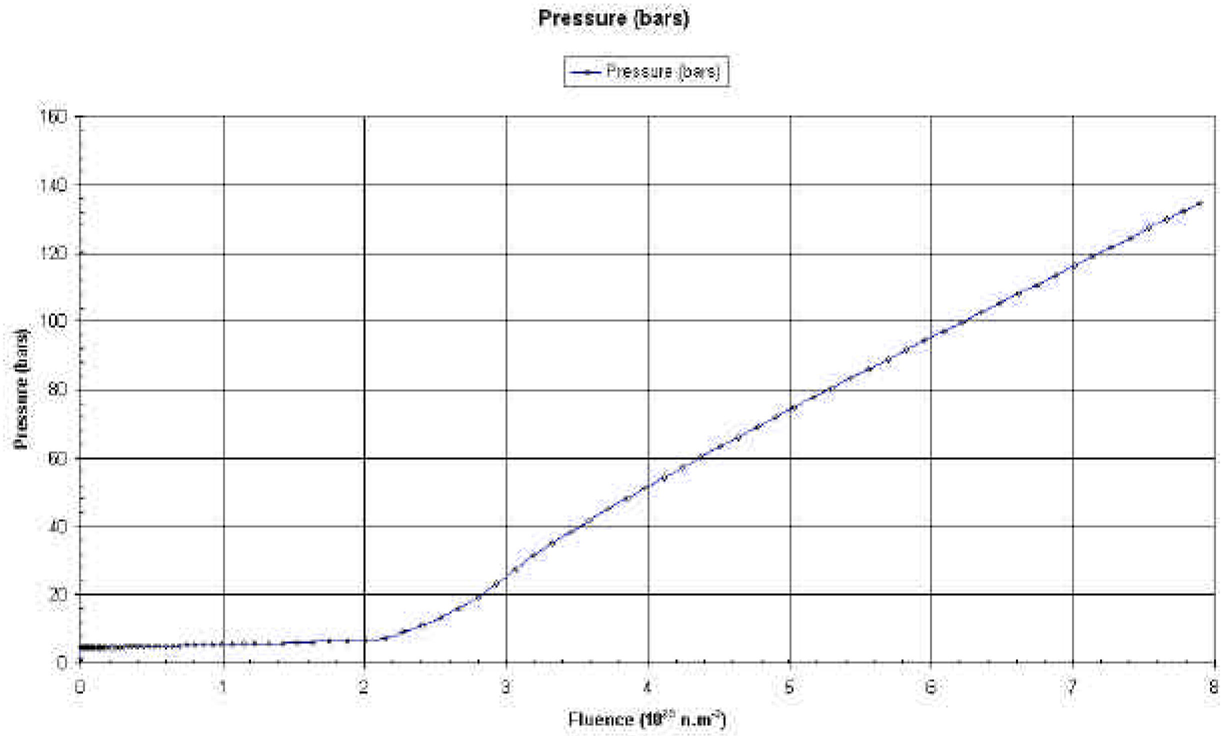
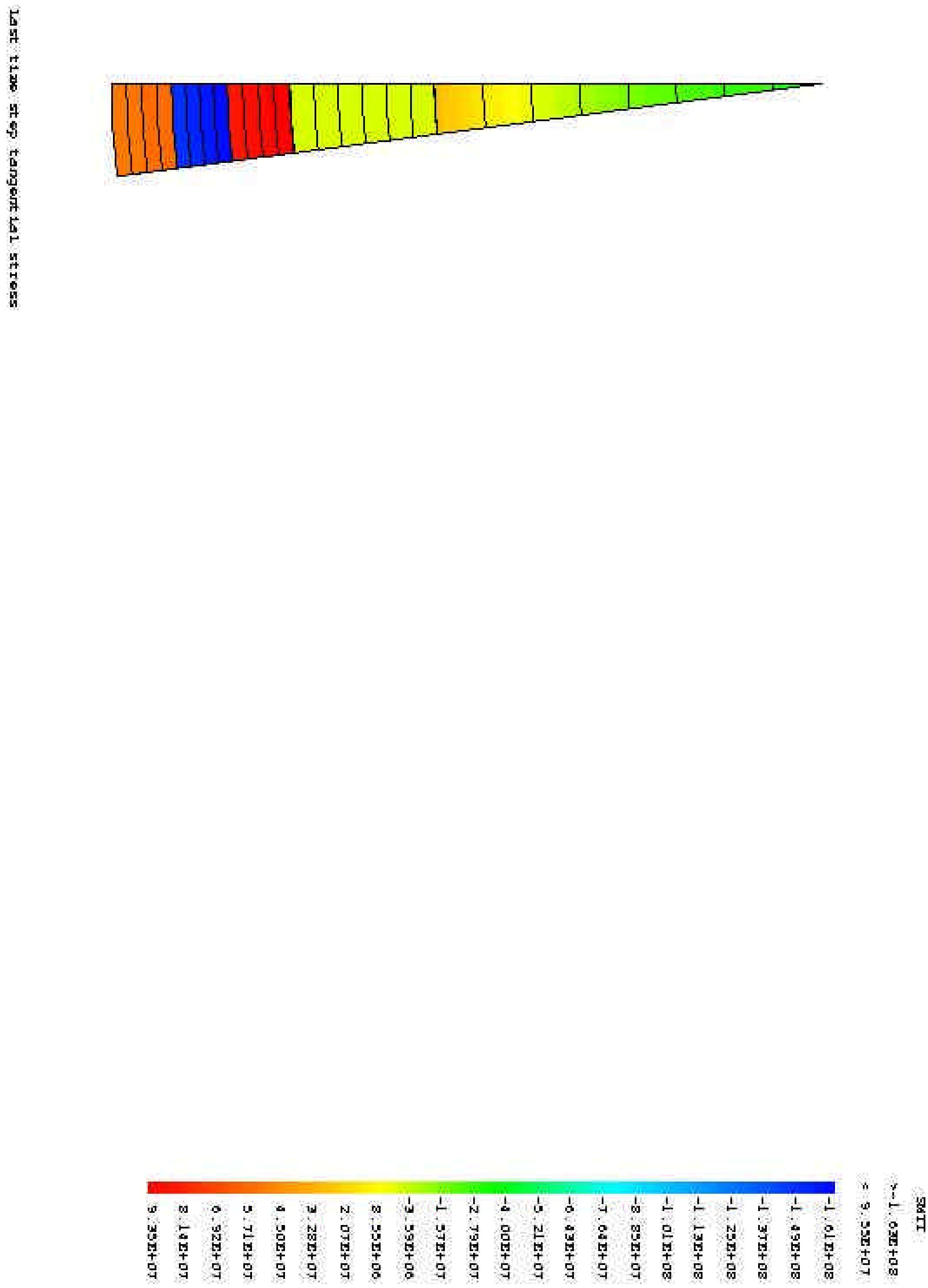



FIGURE 11 : REFERENCE CALCULATION – PRESSURE



<u>FIGURE 12</u> : REFERENCE THERMAL CALCULATION - TEMPERATURE AT T=351 EFPD (K)

FIGURE 13 : REFERENCE MECHANICAL CALCULATION – TANGENTIAL STRESSES AT T=20 EFPD (PA)



## FIGURE 14 : CREEP CONSTANT INFLUENCE – LAYER TANGENTIAL STRESSES

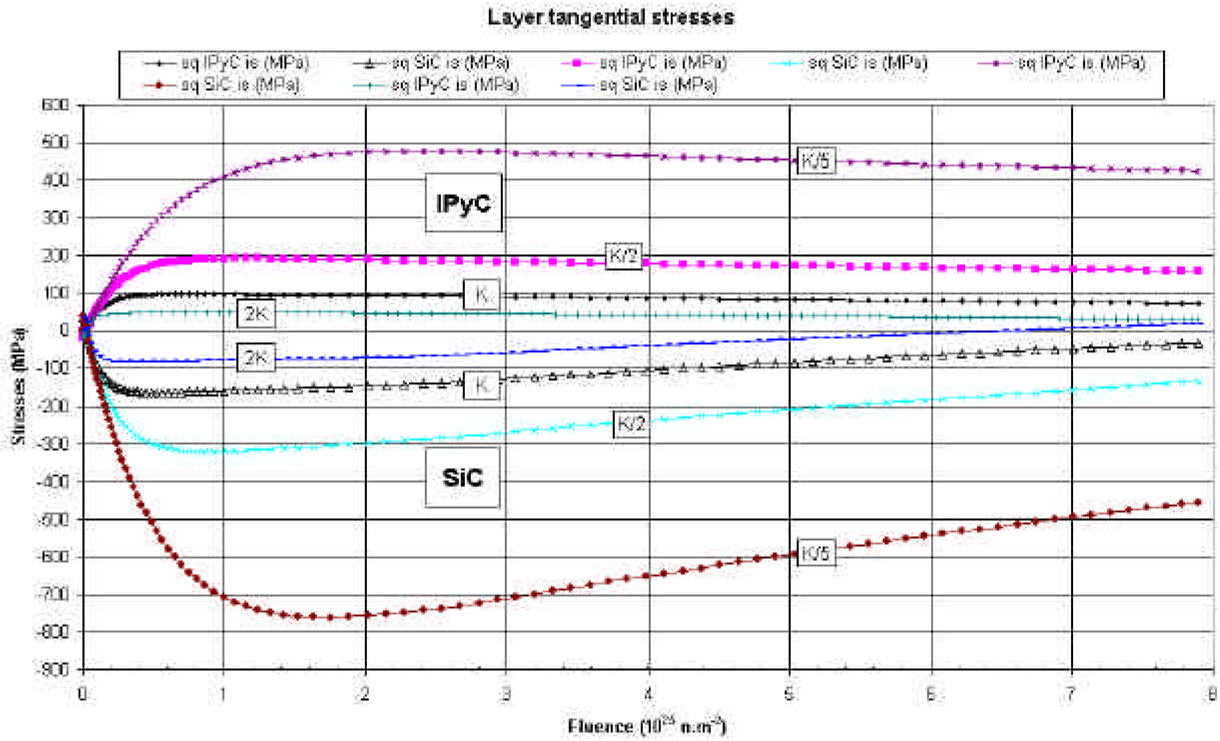
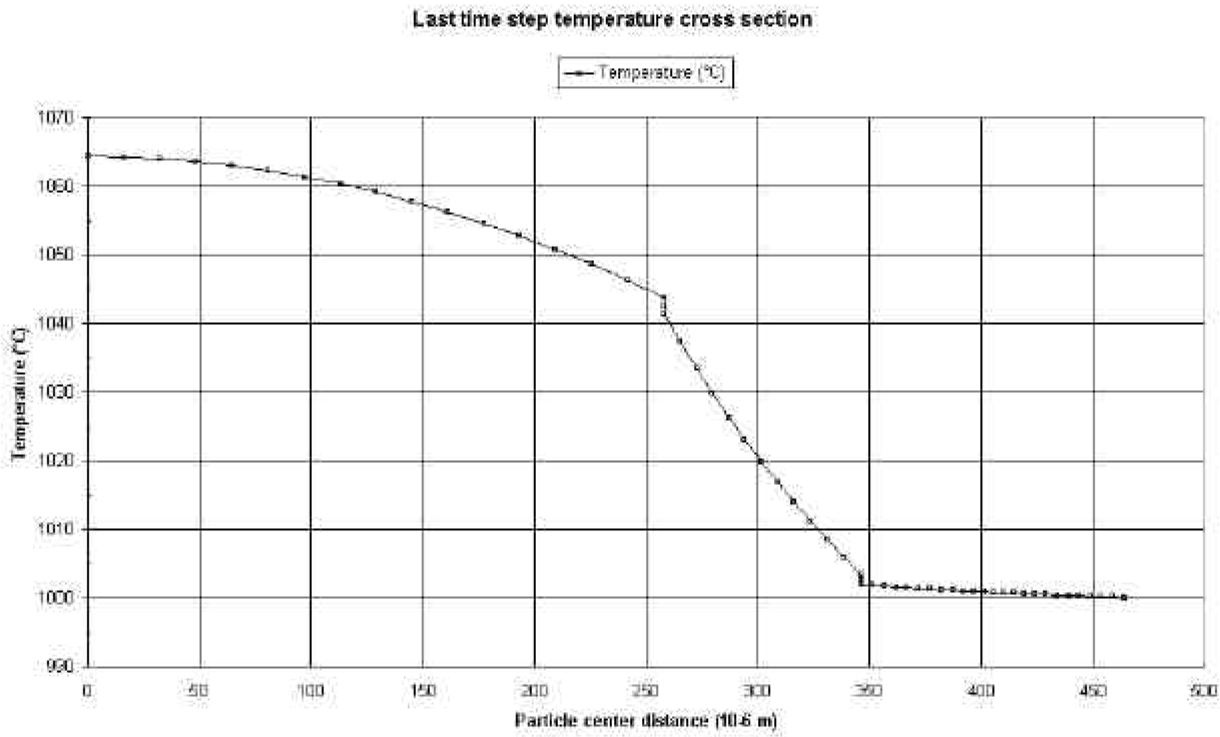


FIGURE 15 : CALCULATION WITH BNFL DATA – THERMAL CALCULATION RESULT



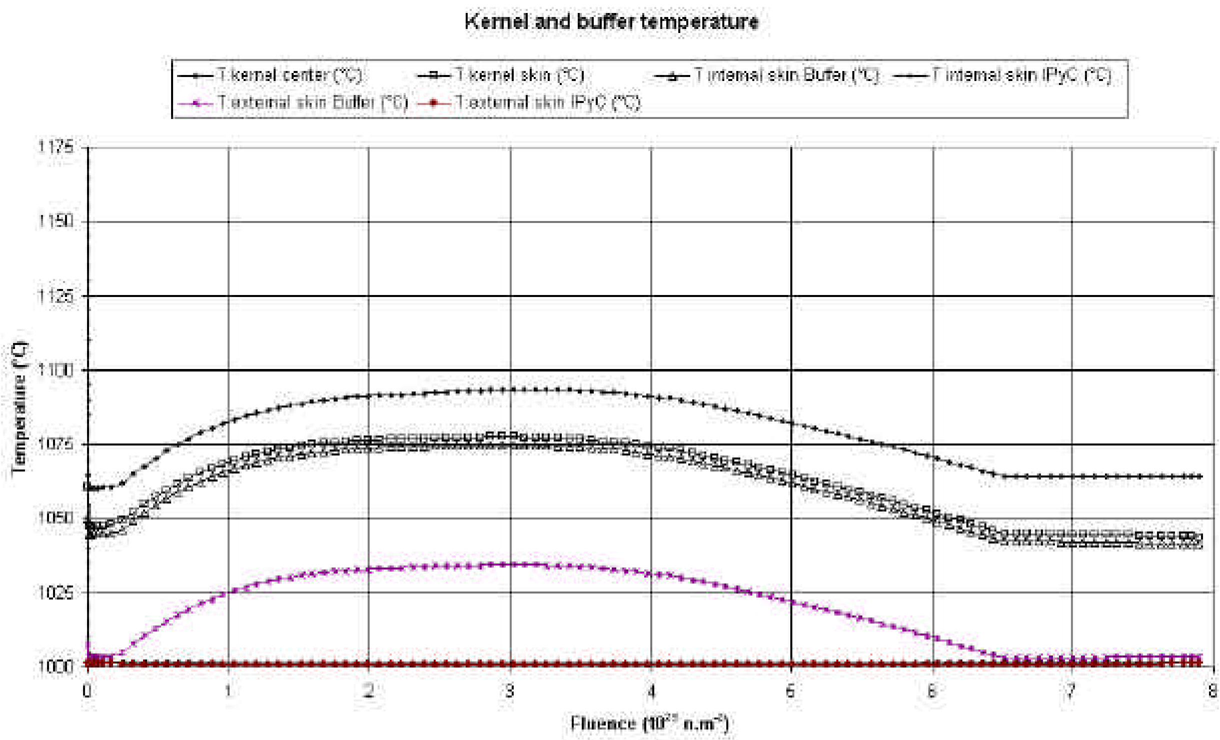
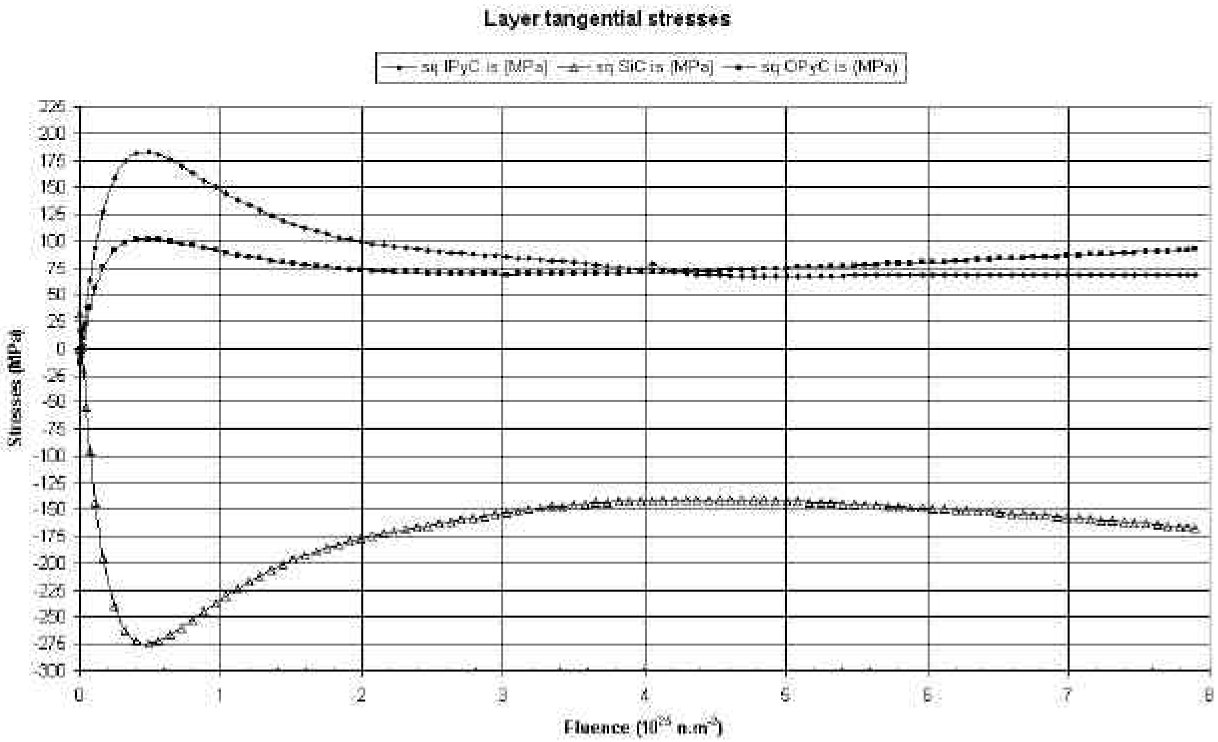



FIGURE 16 : CALCULATION WITH BNFL DATA – LAYER STRESS AND STRAIN



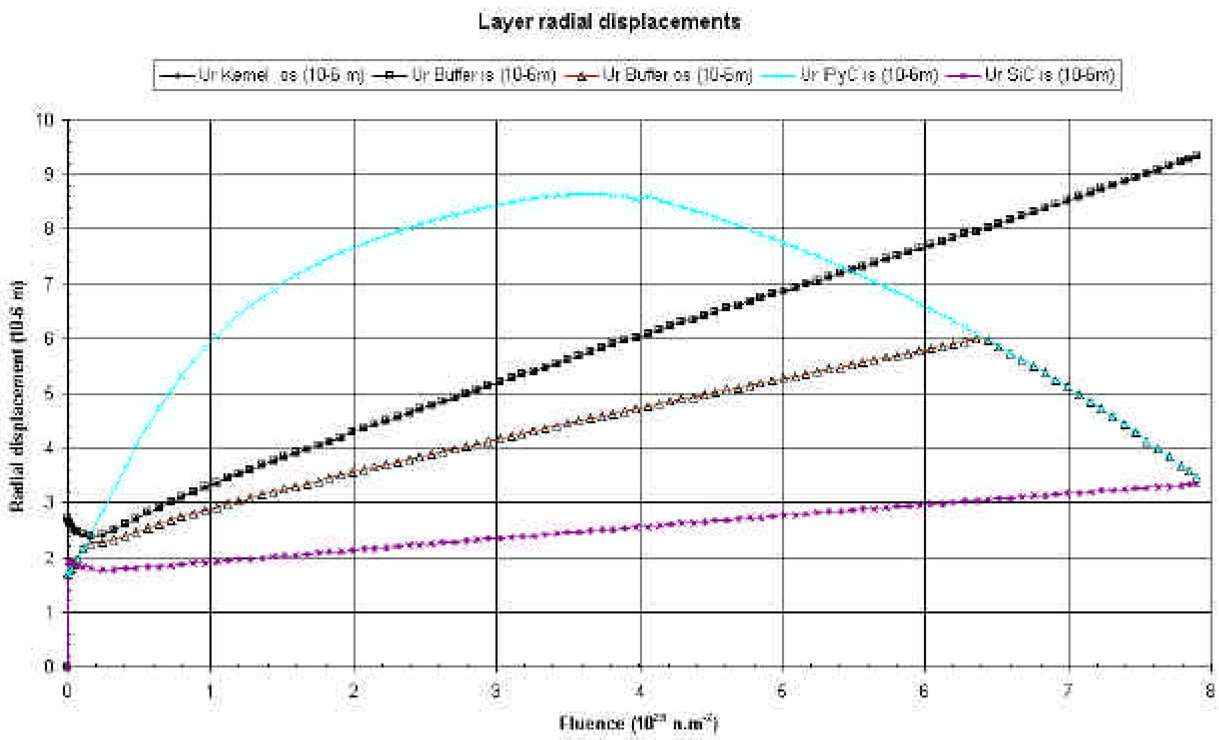
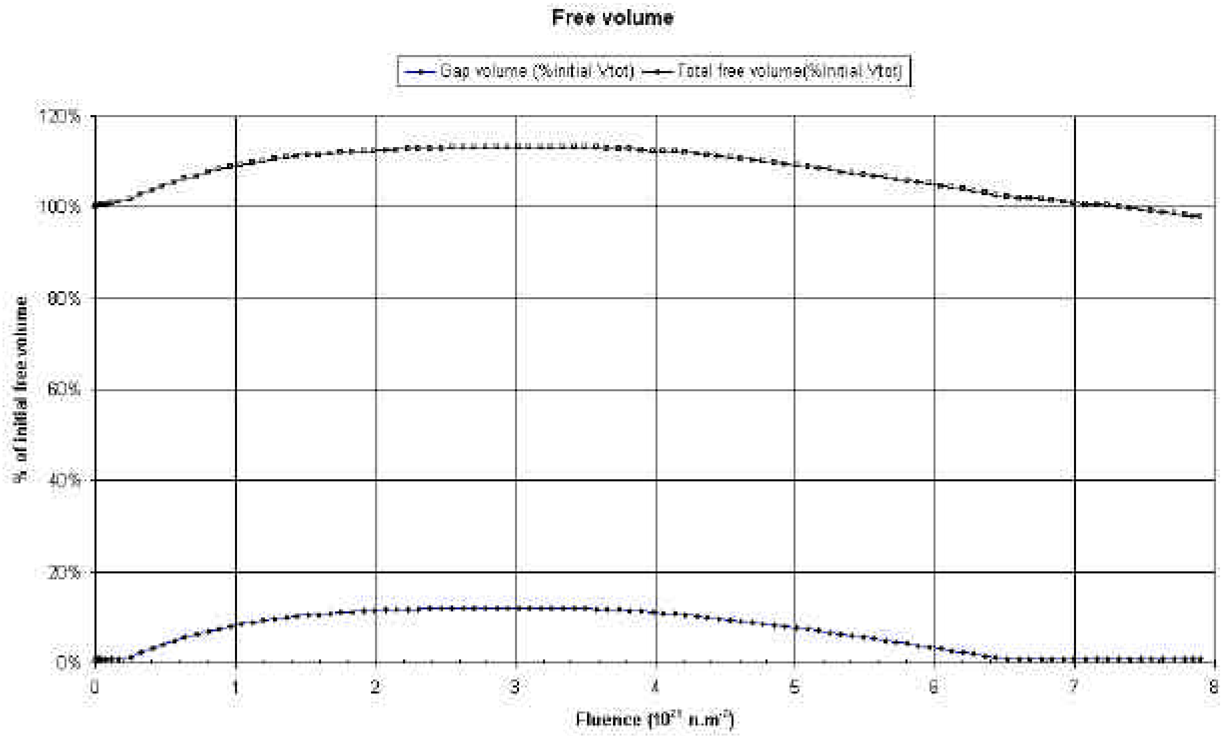



FIGURE 17 : CALCULATION WITH BNFL DATA – FREE VOLUME AND PRESSURE



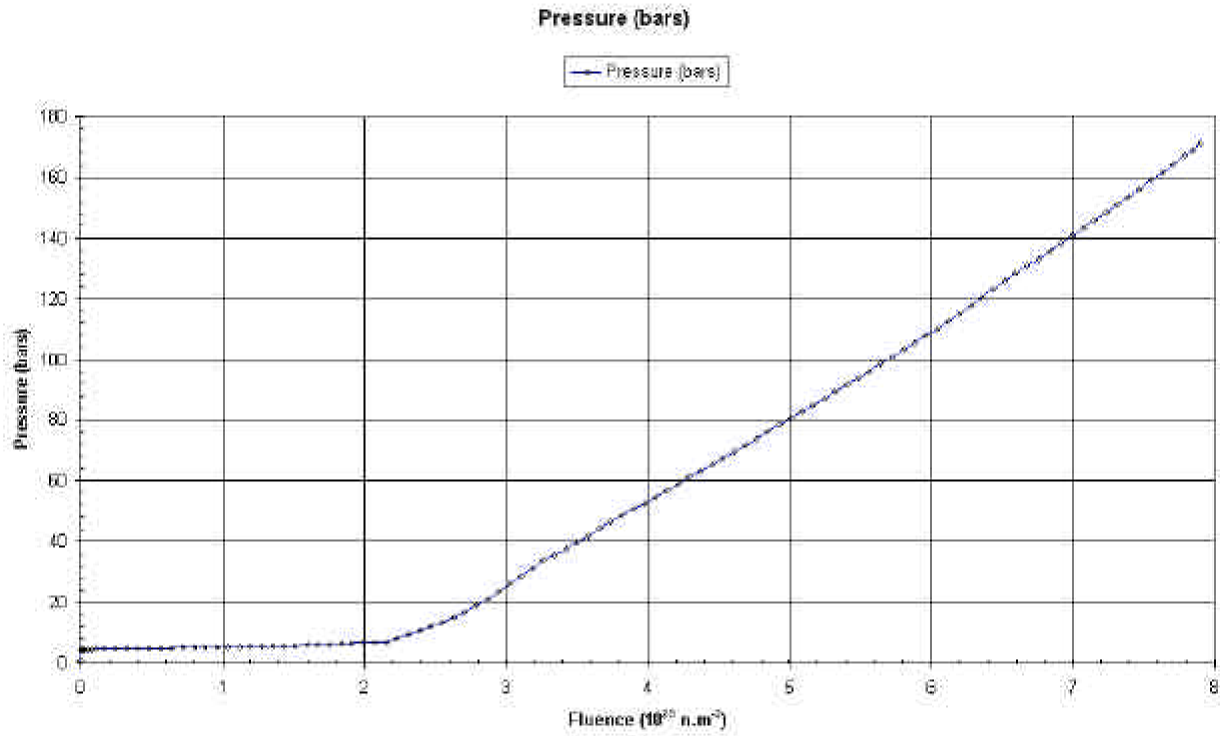
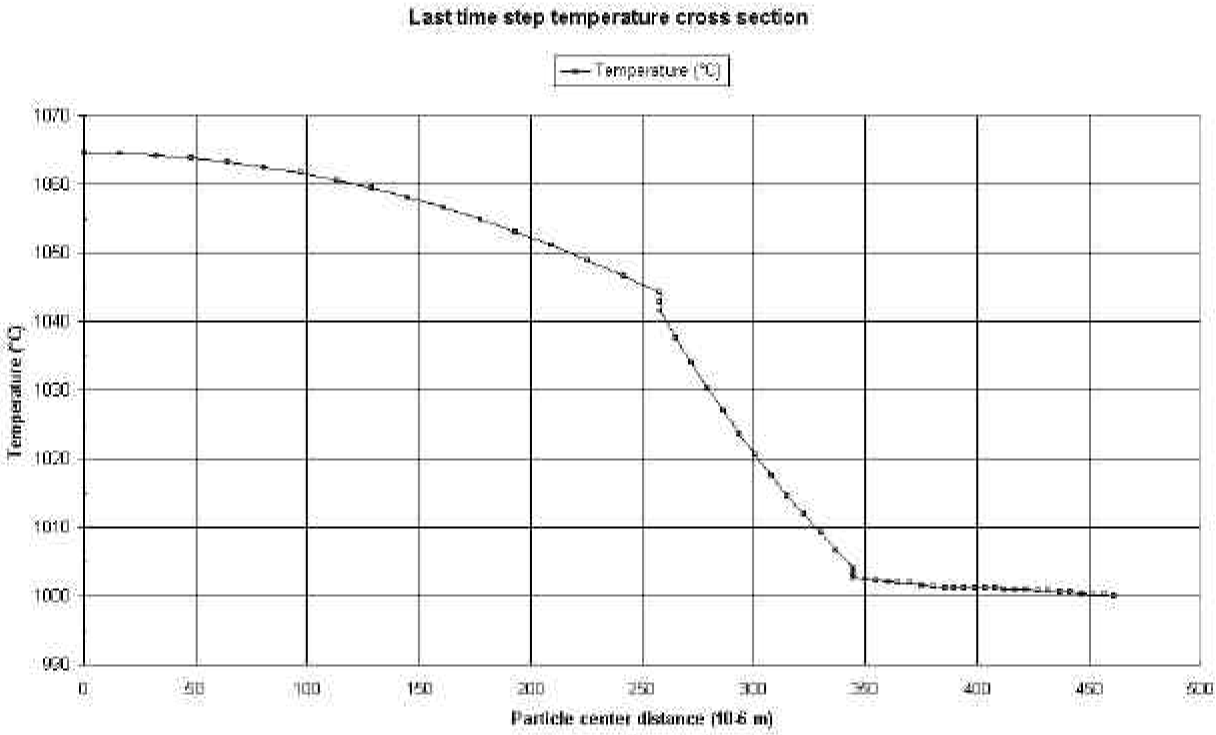



FIGURE 18 : CALCULATION WITH FZJ DATA – THERMAL CALCULATION RESULT



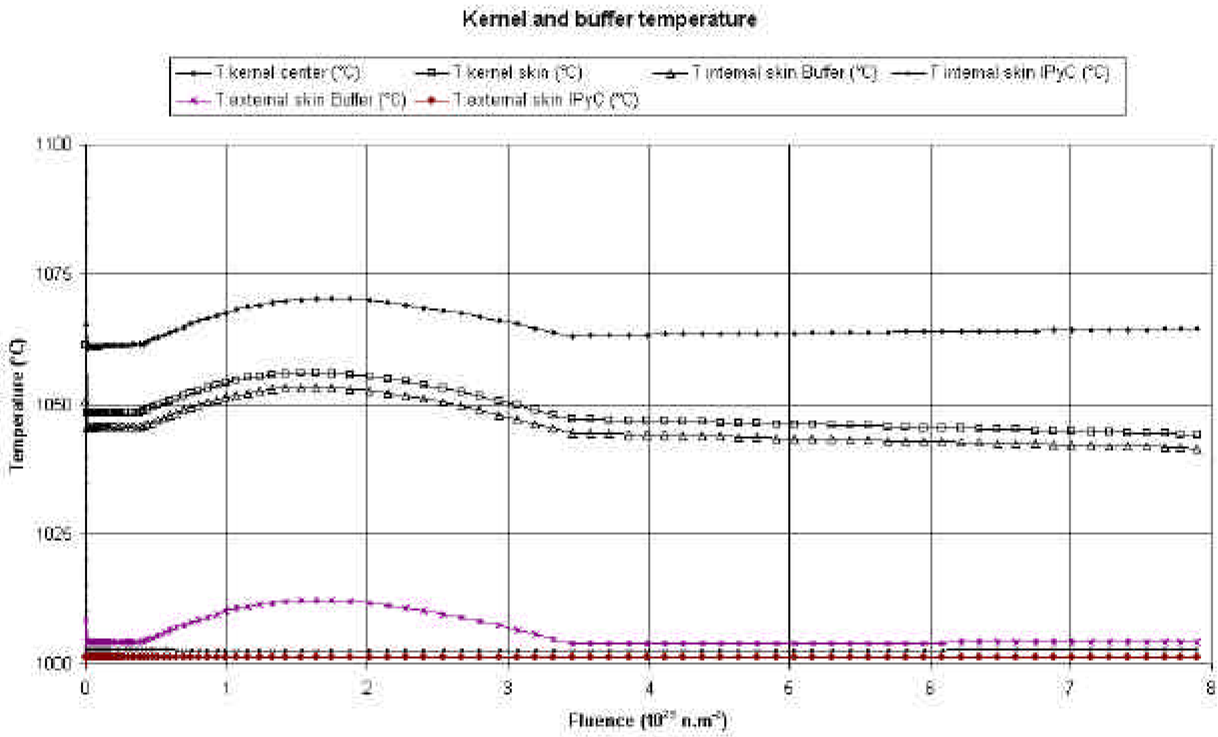
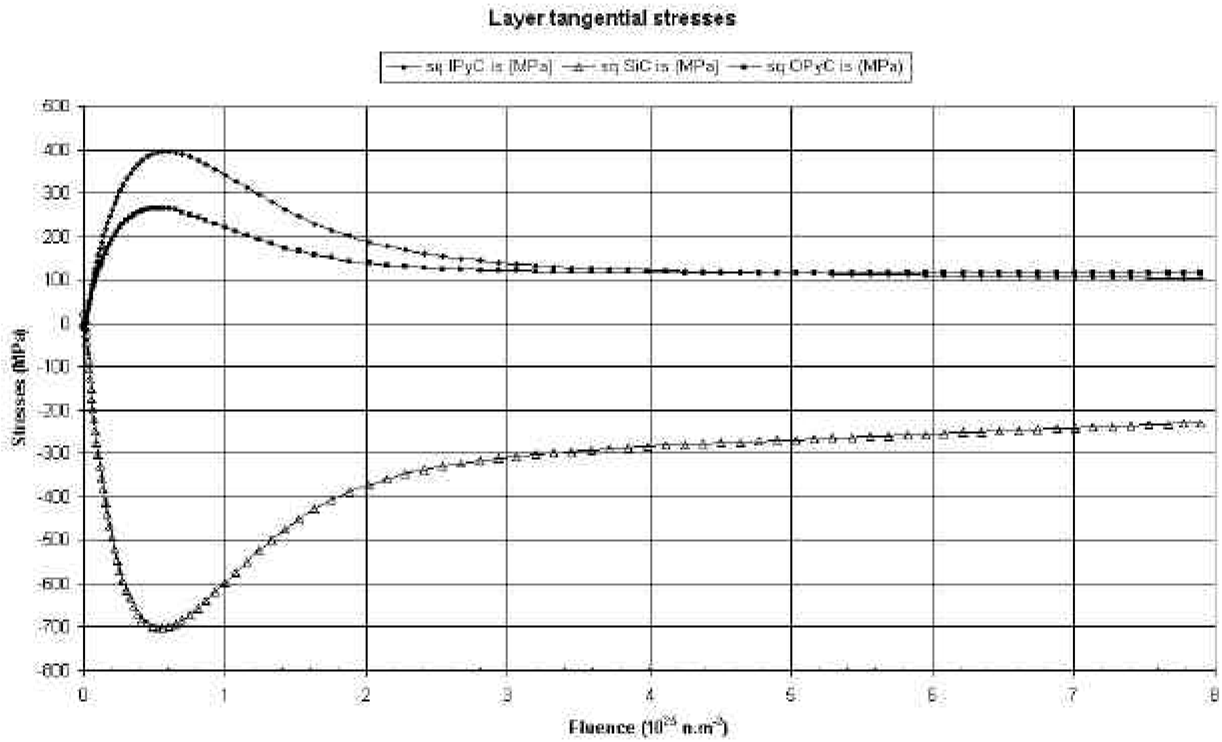



FIGURE 19 : CALCULATION WITH FZJ DATA – LAYER STRESS AND STRAIN



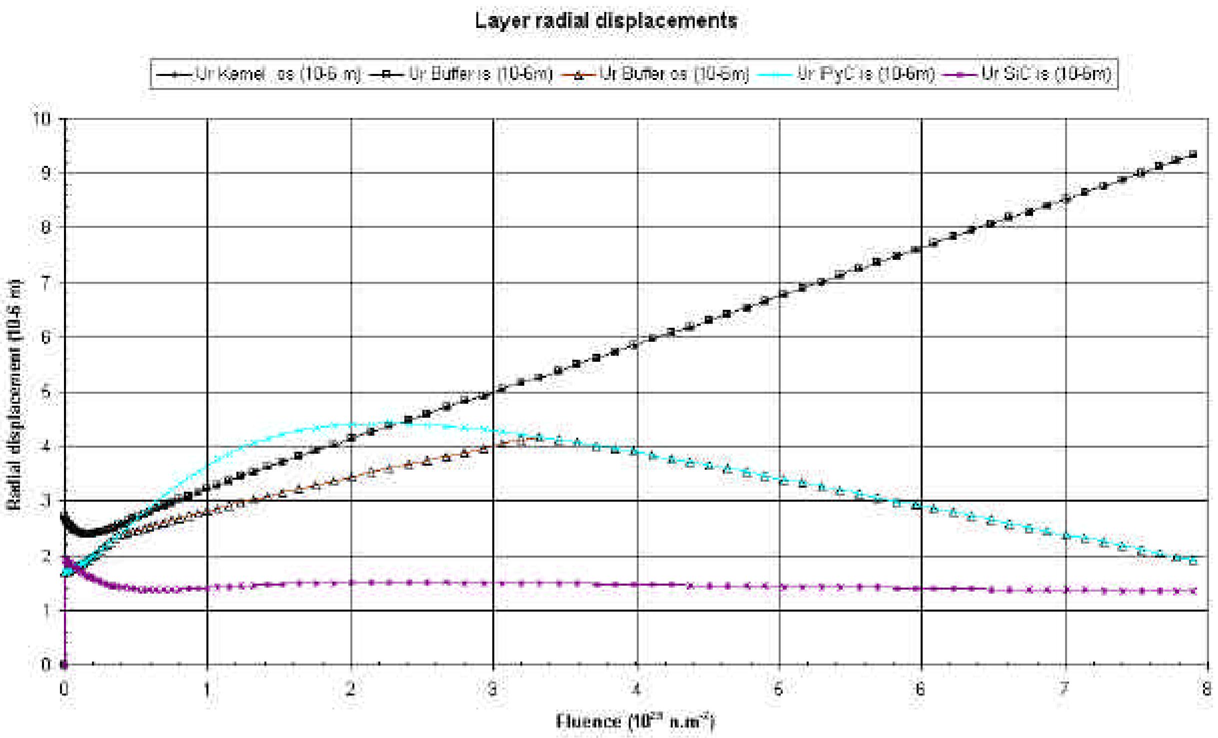
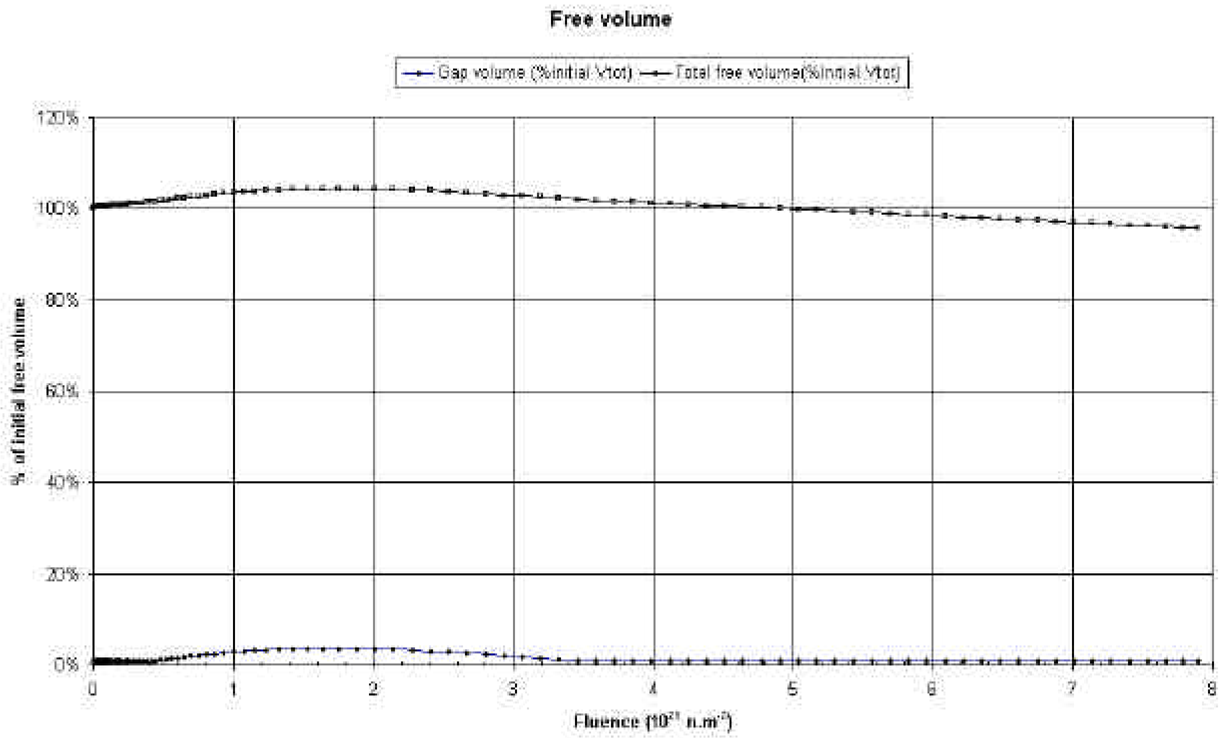
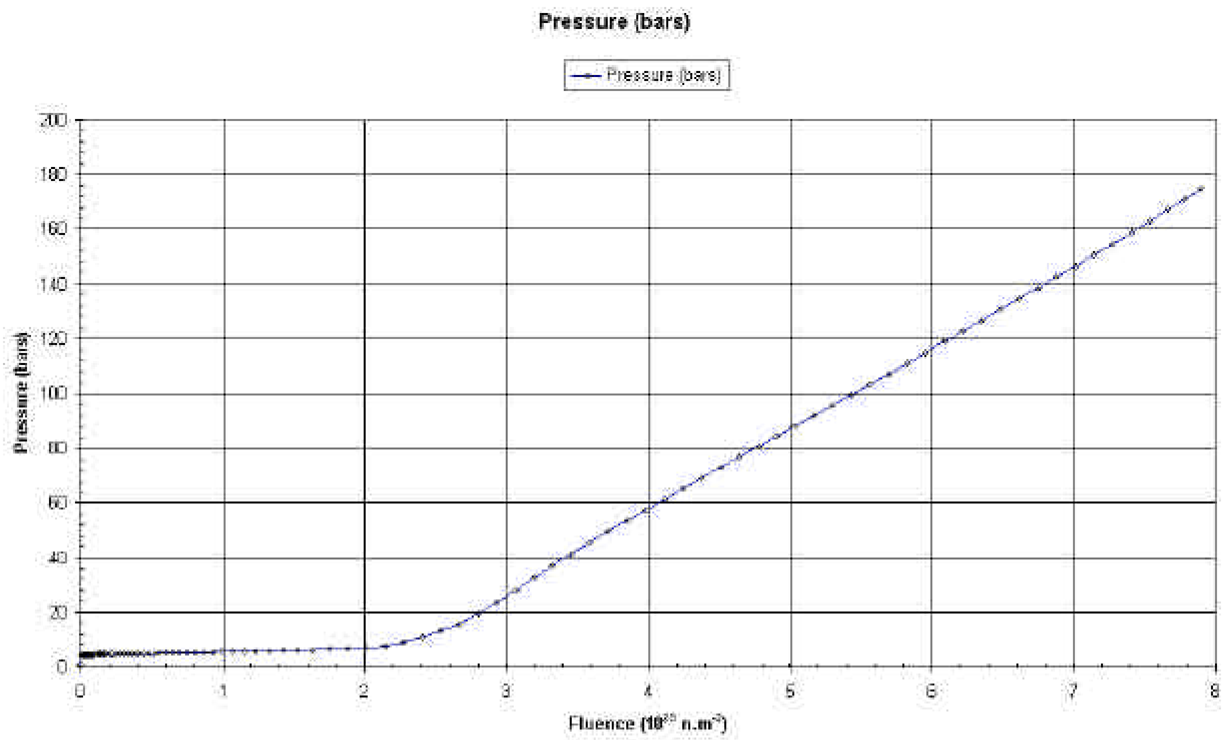



FIGURE 20 : CALCULATION WITH FZJ DATA – FREE VOLUME AND PRESSURE



# LIST OF ANNEXES

## ANNEXE A : REFERENCE CASE ATLAS INPUT DATA

```
************ MAILLAGE  ref1
Type de maillage [mot clé '1D' , '2DCentre' ou '2D'] défaut '2D'
'1D'
Nb de couches (en plus du combustible) (minimum 2 car le chargement de pression interne s'appuie notamment sur
la 2e couche _ max 5 pour la definition des couleurs (opérateur COUL))
4 2
rayon noyau (m) et nb de mailles suivant le rayon
248.5E-6 8
Jeux entre couches (n-1) et n : n (entier) et valeur initiale du jeu (m) (de 0 à n lignes)
1 2.E-7
2 2.E-7
epaisseur minimale du jeu (2.E-7 conseillé)
2.E-7
epaisseur couches (m) et nb de mailles dans l'epaisseur (autant de lignes que de couches)
94.E-6 6
41.2E-6 4
36.E-6 4
40.E-6 4
nombres de portions divisant pi/2 radians du maillage spherique
12
*
************************* MATERIAUX
Noyau : Materiau (mot) et porosité (/)
UO2 0.0137
Noyau : enrichissement (en Pu ou U5) (/), taille des grains (m), stoechiométrie O/M (/)
0.0982 1.E-6 2.008
Fission : Energie et unité [mot:'J/mol' ou eV ou MeV] et nb d'at de gaz produits (/)
200 MeV
Gaz atoms per fission : 'name' and rate (/)
'Xe' 0.301
'He' 0.0
Couches : matériau (MOT) et porosité (/)
LAB 0.5575
LA1 0.177
LA2 0.0
LA1 0.1681
Part des porosités ouvertes dans le noyau et dans le buffer (couche 1)
0. 1.
Gaz interne à la particule de fabrication (mot clé:XE) et pression (en Pa)
'Xe' 1.E5
********* conditions spéciales (voir notice)
* * * *
************ aditional outputs
* * * *
**************   l'historique d'irradiation   ****************
**** Pression extérieure (en Pa)****
1.E5
*** flux neutronique (valeur et MOT clé unité 'n/m2/s' ou 'mol/m2/s', avec les cotes'')3.2E-6 'mol/m2/s'
2.605E+18 'n/m2/s'
*** proba de fission=d[FIMA]/dt (s-1)
4.84726E-09
*** Nombre de pas (autres que t=0), les valeurs au delà ne seront pas lues
2
**** temps max d'une iteration (s) (les iterations rajoutee seront à flu lineairement interpolée)
504800. 1.07
**** mode de calcul du flu neutronique : Mot clé (PROP ou X)
PROP
**** Historique t (s), evolution normée de la proba de fission , et si besoin evolution de la fluence ** dans le
cas ou le mot PROP apparait ci-dessus, il faut 2 valeurs par ligne, sinon il faut 3 valeurs par ligne
0.   293.     * t=0. , pour ce temps seule la température est lue
14400.    1273. 1.0
30326400. 1273. 1.0
```