DE LA RECHERCHE À L'INDUSTRIE

THERMO-CHEMO-MECHANICAL COUPLINGS IN ALCYONE FUEL CODE - APPLICATION TO PELLET CLADDING INTERACTION (PCI)

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MAIN PHENOMENA DURING POWER RAMPS ON UO_2 FUEL

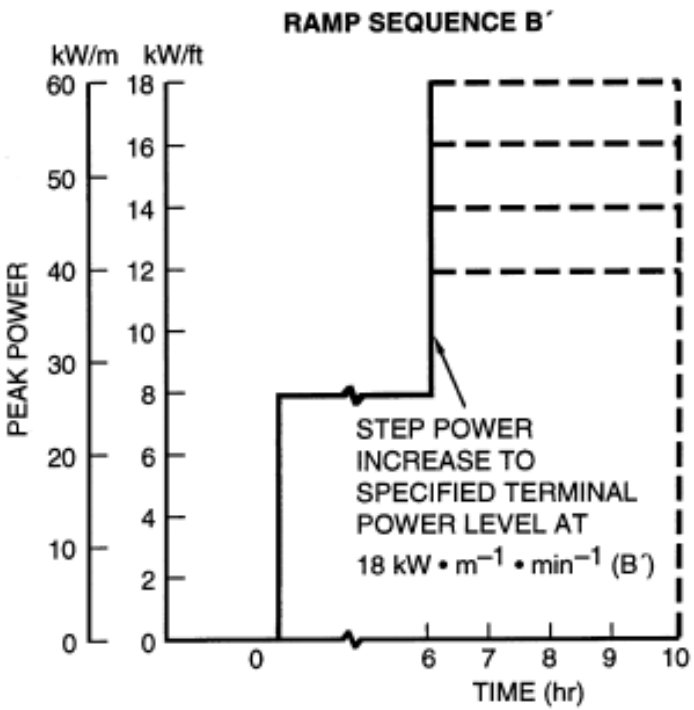
DESCRIPTION OF A POWER RAMP

CONSEQUENCES FOR THE FUEL

CONSEQUENCES FOR THE CLADDING

DESCRIPTION OF A POWER RAMP

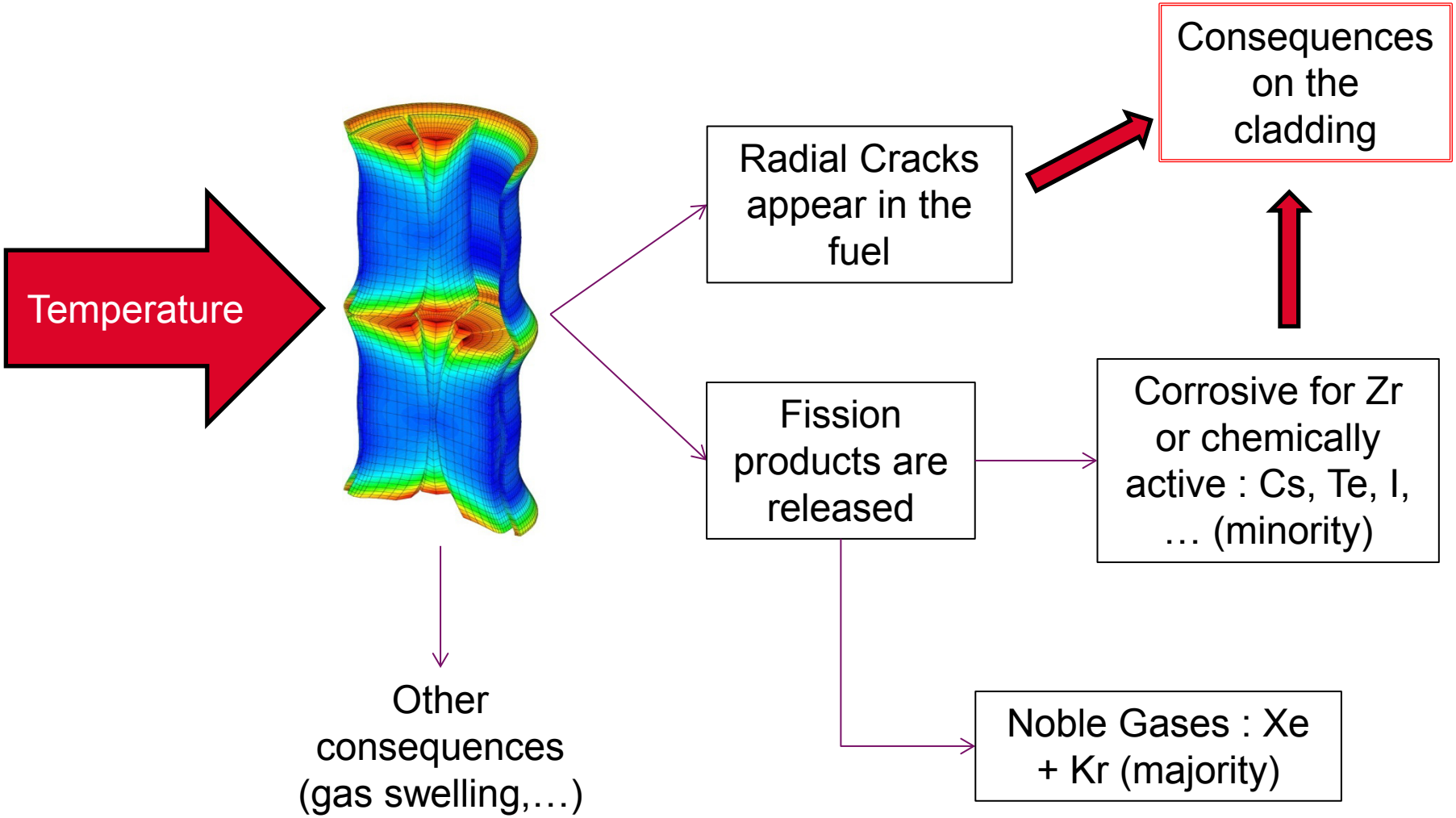
Description of a power ramp on a fuel rod :



- Incidental 4-Step scenario :
  - A conditioning step at ~200 W/cm
  - A power transient at about ~ 100 W/cm/min
  - A holding time at P>400W/cm
  - A return at 0 W/cm
- First consequence for the pellet : strong increase of the central temperature with an almost constant clad temperature
  A more than 300 K/mm temperature gradient in the pellet

J.H. Davies et al. JNM 270, 1999, pp87-95

CONSEQUENCES FOR THE FUEL



CONSEQUENCES FOR THE CLADDING

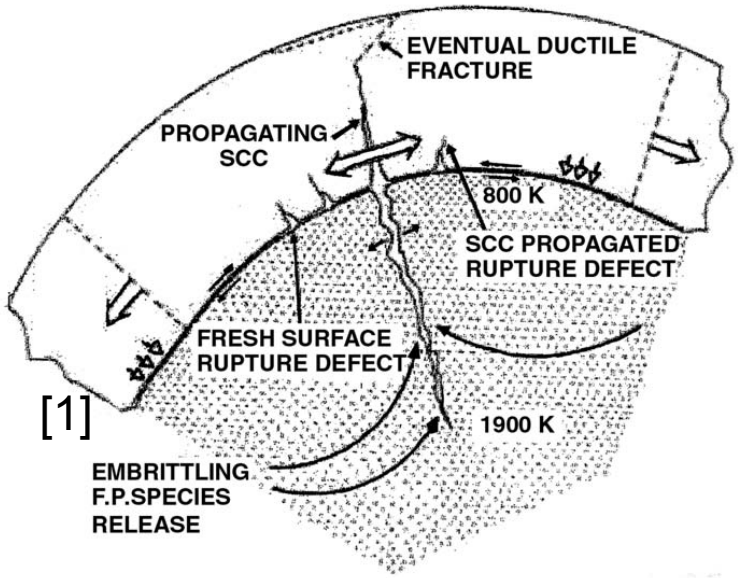
Radial Cracks appear in the fuel

High local stresses in front of the fuel cracks apperture

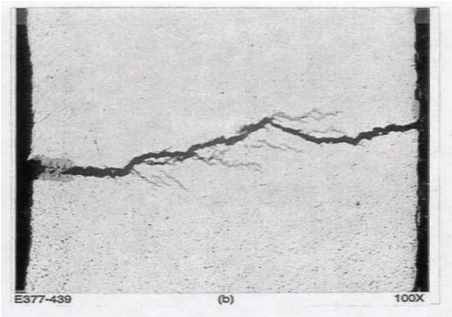
Direct path from the pellet center to the cladding

I-SCC cracks initiation on the internal face of the cladding

Corrosive for Zr or chemically active : Cs, Te, I, … (minority) release



[1]



Condition for initiation of I-SCC cracks :

- High stresses on the cladding
- Quantity of Iodine :
  - Surfacic concentration of 10^{-3} mg/cm² [3]
    OR
  - P_{I2}>50 Pa [2]

[1] IZNA-6 special report. ANT international, 2006
[2] C. Anghel et al. Proceedings of Top Fuel 2010 Orlando, Florida, USA, September 26-29, 2010
[3] P. Bouffioux et al. Journal of Nuclear Materials, vol. 87, pp. 251-258, 1979.

ALCYONE AND ANGE FUEL CODES

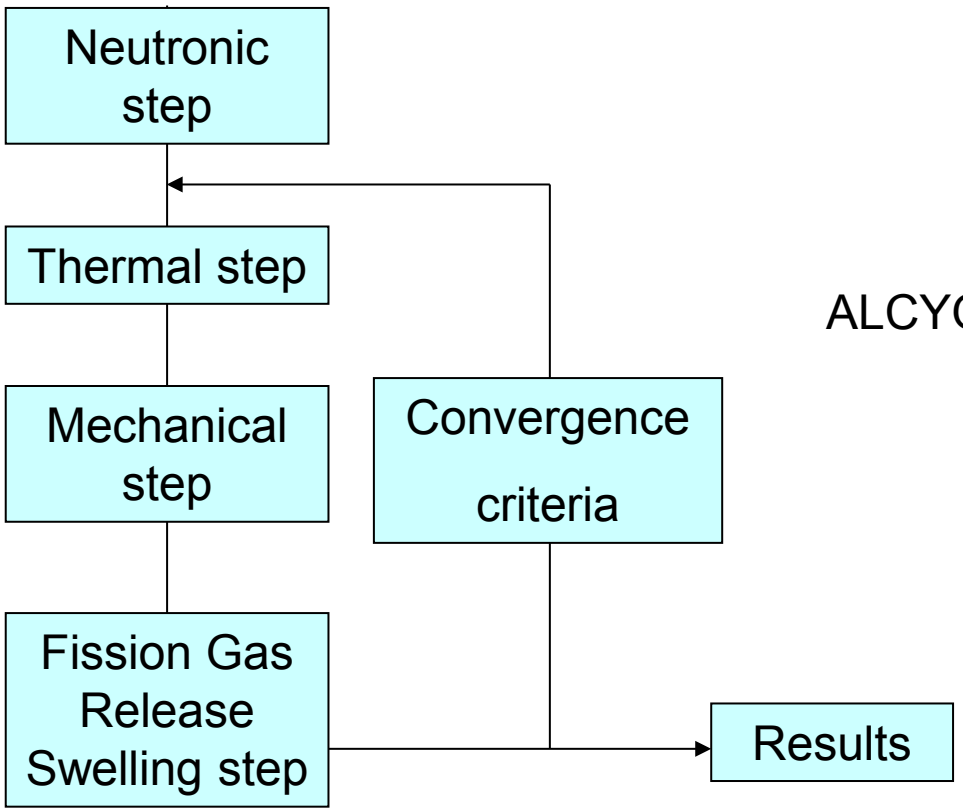
ALCYONE : THERMO-MECANICAL FUEL CODE

ANGE : THERMOCHEMICAL FUEL CODE

ALCYONE-ANGE COUPLING SCHEME

ALCYONE : THERMO-MECANICAL FUEL CODE

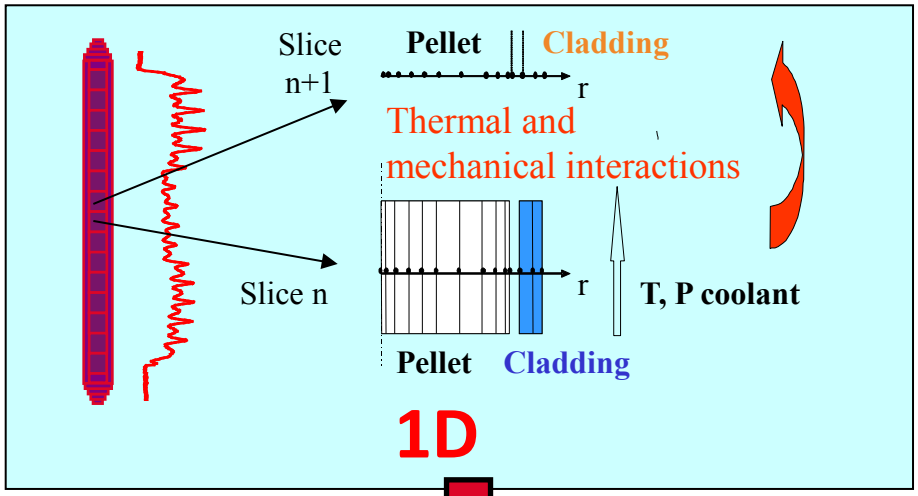
ALCYONE : the CEA thermo-mechanical code dedicated to fuel behavior modeling in normal, incidental or accidental situations.

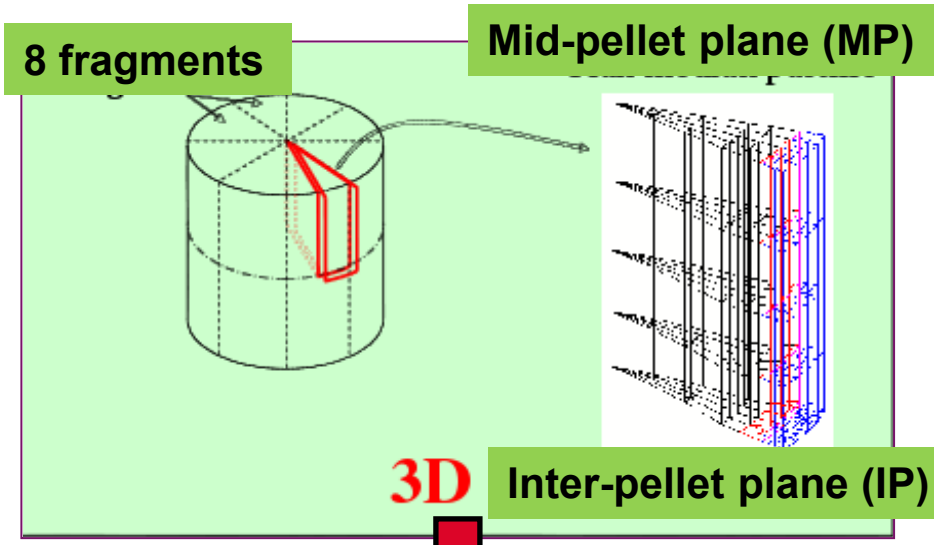


ALCYONE calculation scheme

B. Michel et al. Comprehensive Nuclear Materials, 2012, pp 677-712

ALCYONE : THERMO-MECHANICAL FUEL CODE





- Fuel rod discretized in axial slices
- Axial slices **are divided in annular rings**
- On each node. a calculation of **T, P, BU, swelling, …**
- A thermo-hydraulic calculation is performed on the full rod.
- Provides **input data for 3D calculations** (T, P, …)

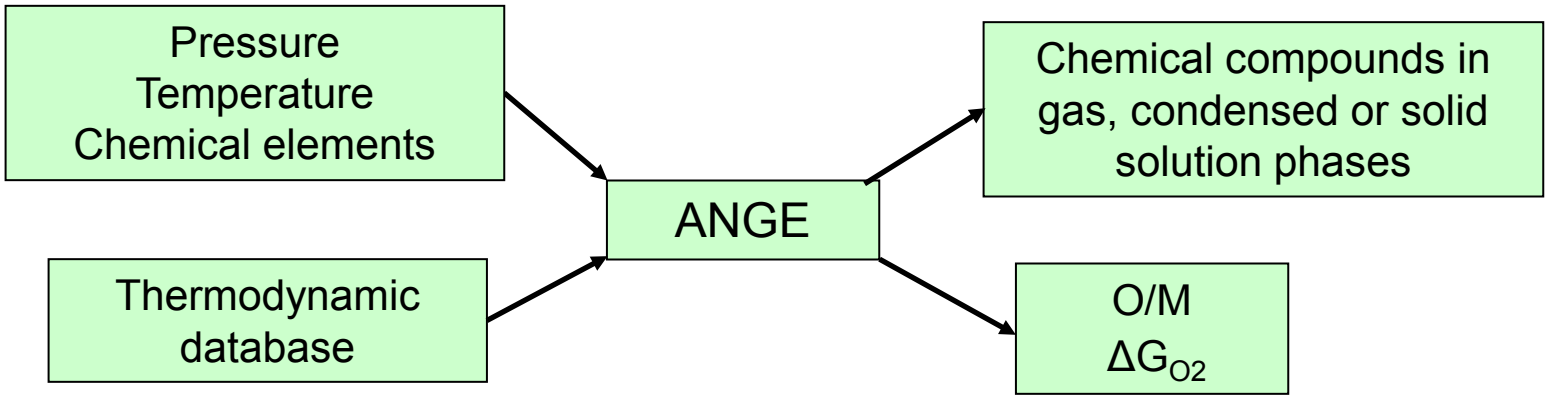
- **1/32 of pellet** is considered thanks to symmetry (one quarter of a pellet fragment)
- **1 IP et 1 MP** are modelled
- **Exact geometry** of the pellet (dishing, chamfer,…)
- **Pellet cladding interaction** simulated by a friction model

B. Michel et al. Comprehensive Nuclear Materials, 2012, pp 677-712

ANGE : THERMOCHEMICAL FUEL CODE

Thermochemical fuel code

- ANGE is a code developed by the CEA and EDF, adapted to describe the chemical behavior of irradiated fuel.
  - Based on a minimisation of the free energy of the system (SOLGASMIX-like solver)
  - Contains a description of the solid solution of UO_2 with its fission products (Lindemer and Besmann)
  - Approach validated by J.C. Dumas in his PhD (1995)



J.C. Dumas. PhD thesis. Institut National Polytechnique, Grenoble, France, 1995.
T. Lindemer and T. Besmann. Journal of Nuclear Materials, vol. 130, pp 489-504, 1985.
T. Lindemer and T. Besmann, vol. 130, pp 473-488, 1985.
T. Lindemer and T. Besmann, Journal of American Ceramic Society, vol. 69, pp 867-876, 1986.

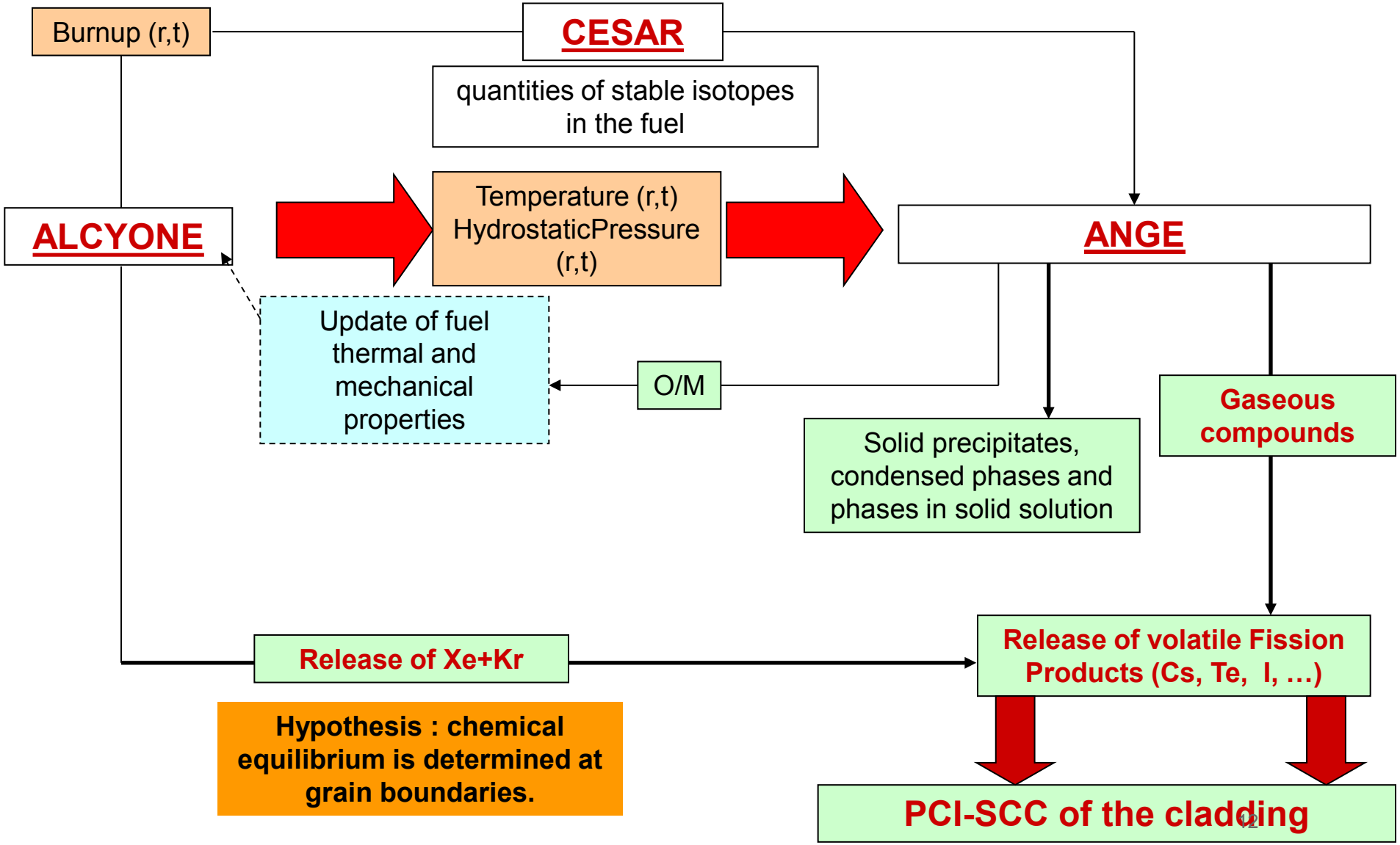
Chemical elements and quantities considered

Element(s)	Generation (mol/at%/molUO2)	Family
Xe + Kr Cs + Rb I + Br Te + Se	$3.05815.10^{-3}$ $1.69905.10^{-3}$ $1.30854.10^{-4}$ $3.02223.10^{-4}$	Fission gases and volatile fission products
Ba + Sr Zr + Nb	$1.38152.10^{-3}$ $2.62295.10^{-3}$	Stable oxydes
Mo	$2.33462.10^{-3}$	
Ru + Tc + Rh Pd	$2.44048.10^{-3}$ $1.02040.10^{-3}$	Metallic fission products
Ce Eu + Sm La + Y Gd + Nd + Pm Pr	$1.23950.10^{-3}$ $3.80844.10^{-4}$ $9.31065.10^{-4}$ $1.91866.10^{-3}$ $5.29694.10^{-4}$	Fission products in solid solution in UO2

- Estimation of the abundance of fission products based on calculations performed with the depletion code CESAR
- A set of empirical correlations give the quantity of elements depending on the burnup
- The chemical elements sharing the same behavior are mixed together

J.C. Dumas. PhD thesis, Institut National Polytechnique, Grenoble, France, 1995.
J.-M. Vidal et al. Waste Management 2012, Phoenix Arizona, USA, 2012.

ALCYONE-ANGE COUPLING SCHEME



RESULTS FOR A SHORT HOLDING TIME POWER RAMP AND COMPARISON TO EXPERIMENTAL OBSERVATIONS

POWER RAMP CALCULATED

CS, I AND TE COMPOUNDS CREATED AT THE BEGINNING OF THE HOLDING TIME

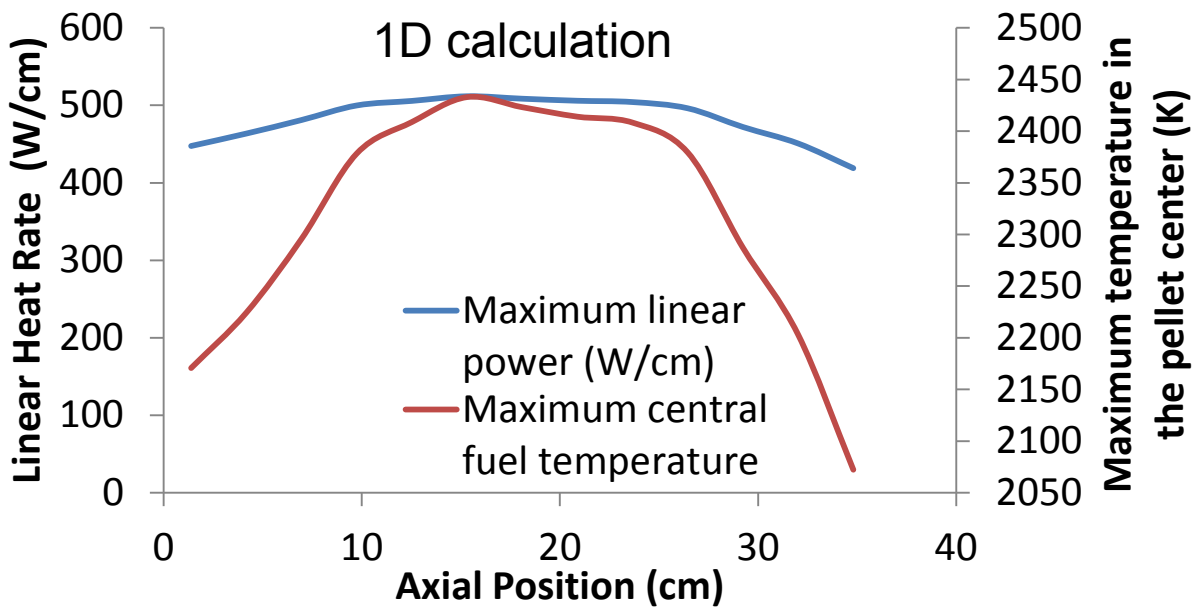
RESULTS ON I, CS AND TE RELEASE COMPARISON TO SIMS OBSERVATIONS

POWER RAMP CALCULATED

Irradiation time	3 cycles
Average cycle power (W/cm)	178-260-214
Cladding	Zy4
Fuel	UO_2
^{235}U content	4.5%
Maximum power during ramp	520 W/cm
Holding time	1min30
Xe+Kr gas release	3.8%

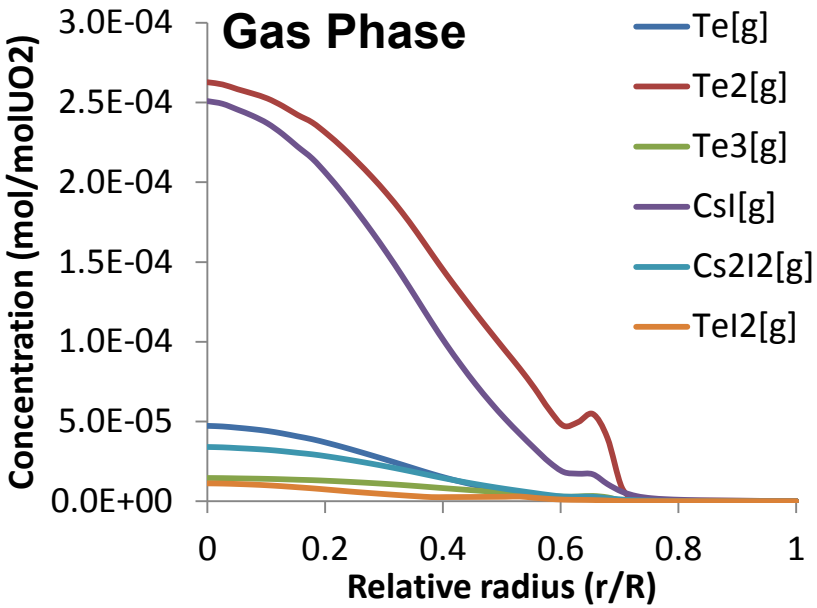
SIMS measurements on Cs, Te and I were performed on a pellet that experienced the maximum power during the ramp.

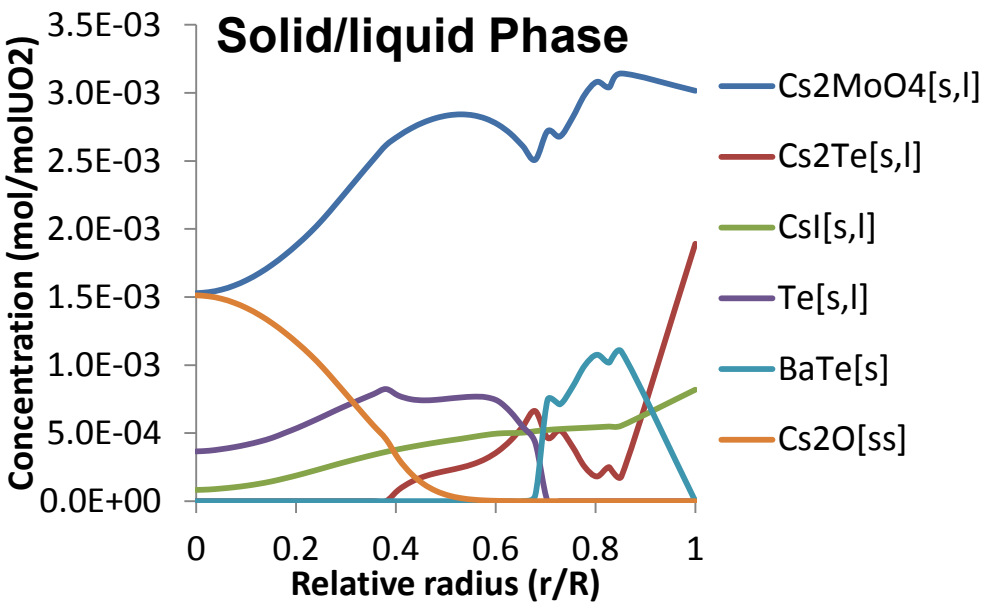
The clad examination revealed I-SCC cracks but no failures.



L. Desgranges et al, Journal of Nuclear Materials, vol. 437, pp. 409-414, 2013.

CS, I AND TE COMPOUNDS CREATED AT THE BEGINNING OF THE HOLDING TIME





The major gaseous compounds created are :

- Te2(g)
- CsI(g)

Minor gaseous compounds involving I are :

- $Cs_2I_2(g)$
- $TeI_2(g)$

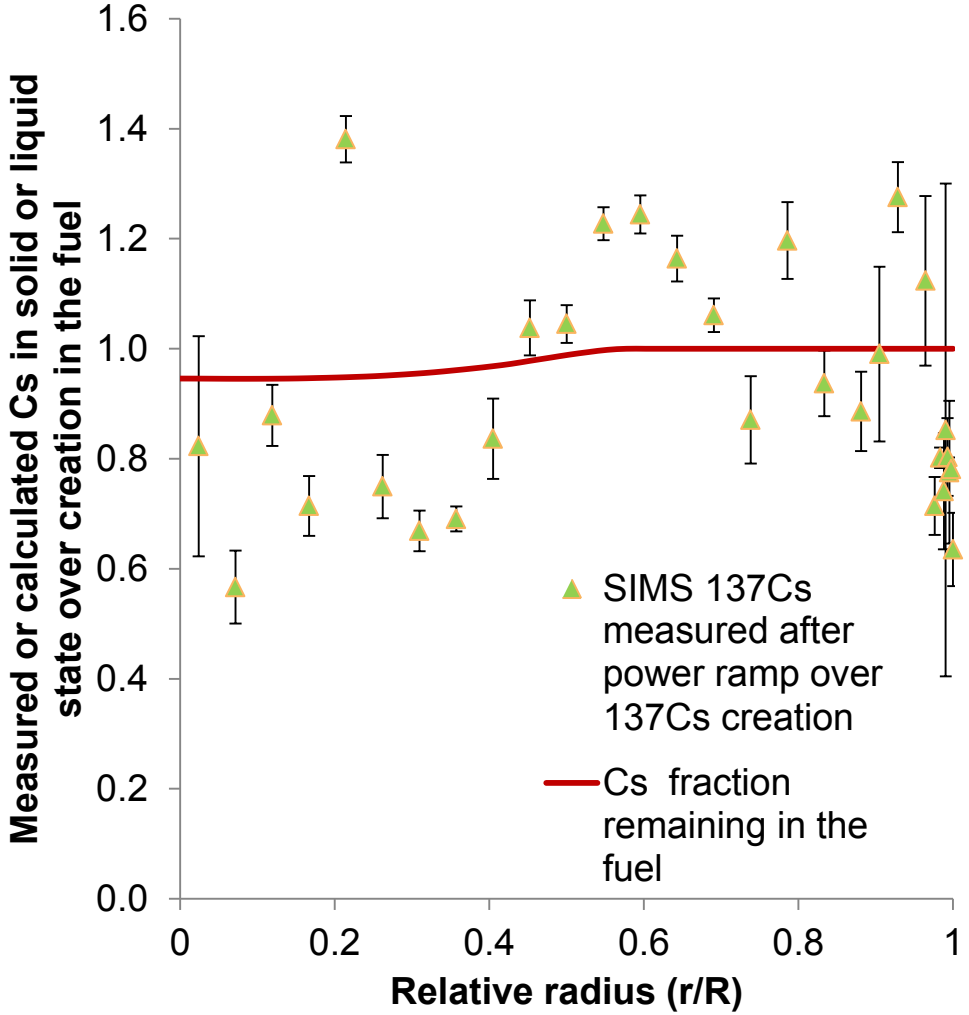
The main compounds in condensed phase or solid solution involving Cs, Te and I are :

- CsI(s,l)
- $Cs_2O(ss)$
- $Cs_2MoO_4(s,l)$
- $Cs_2Te(s,l)$

All these compounds include Cs, leading to a large amount of Cs in solid or liquid phase, It will limit its release.

RESULTS ON I, CS AND TE RELEASE COMPARISON TO SIMS OBSERVATIONS

- Comparison of the Cs, Te and I solid and liquid fractions at the end of the calculation with after-ramp SIMS radial measurements (Cs, Te or I measured/creation)



High dispersion of the Cs radial profile in the SIMS measurements makes any conclusion difficult

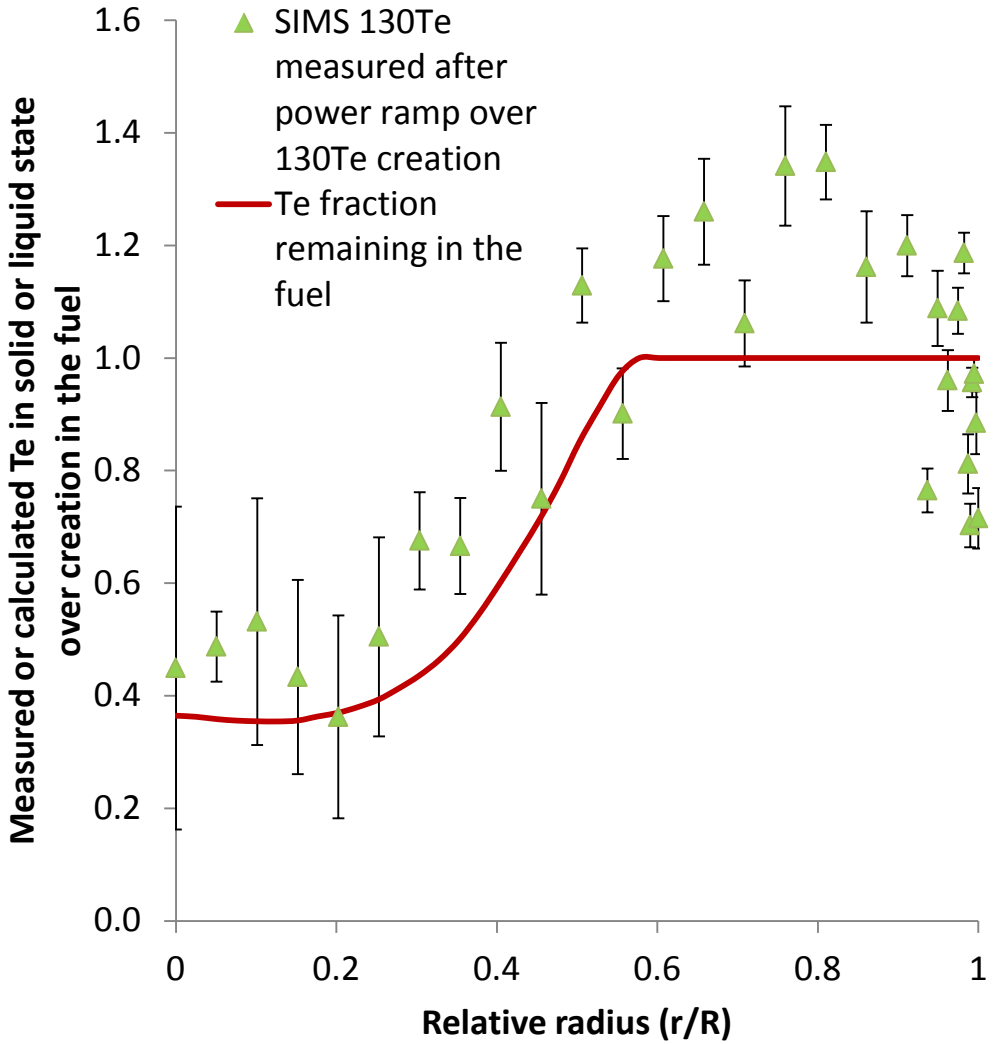
A low fraction of Cs seems to be released

There could be Cs radial redistribution (not modelled yet)

Oxygen redistribution (not modelled yet) can modify chemical equilibrium leading to a higher Cs release

RESULTS ON I, CS AND TE RELEASE COMPARISON TO SIMS OBSERVATIONS

- Comparison of the Cs, Te and I solid and liquid fractions at the end of the calculation with after-ramp SIMS radial measurements (Cs, Te or I measured/creation)



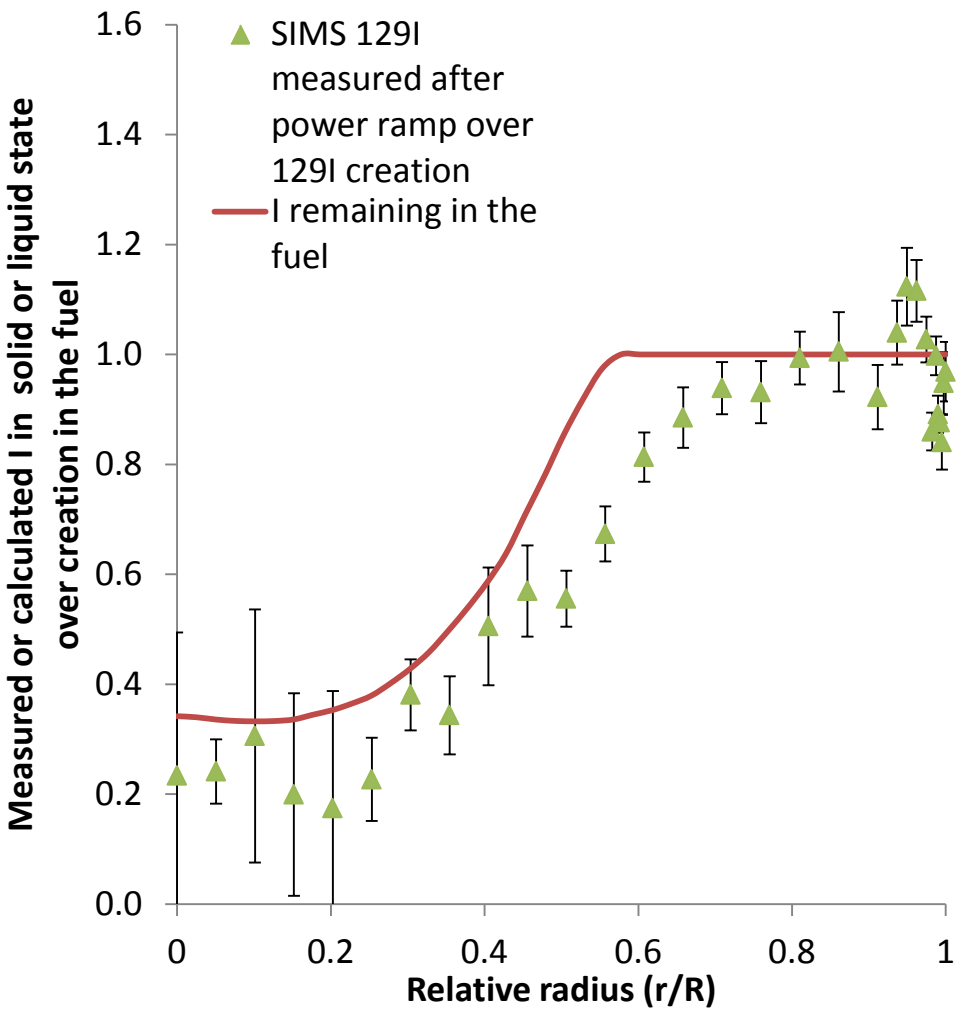
The Te release fits well the experimental measurements at the center of the pellet.

The Te accumulated at the periphery might be the result of a condensation of the Te released from the fuel center.

This hypothesis has to be investigated to improve the modelling of the fission product release.

RESULTS ON I, CS AND TE RELEASE COMPARISON TO SIMS OBSERVATIONS

- Comparison of the Cs, Te and I solid and liquid fractions at the end of the calculation with after-ramp SIMS radial measurements (Cs, Te or I measured/creation)



The I release fits well the experimental measurements at the center of the pellet but is underestimated at mid-radius of the pellet.

The Iodine accumulated at the periphery can result from a condensation mechanism on the cold part of the fuel, as for Te.

This hypothesis needs to be investigated.

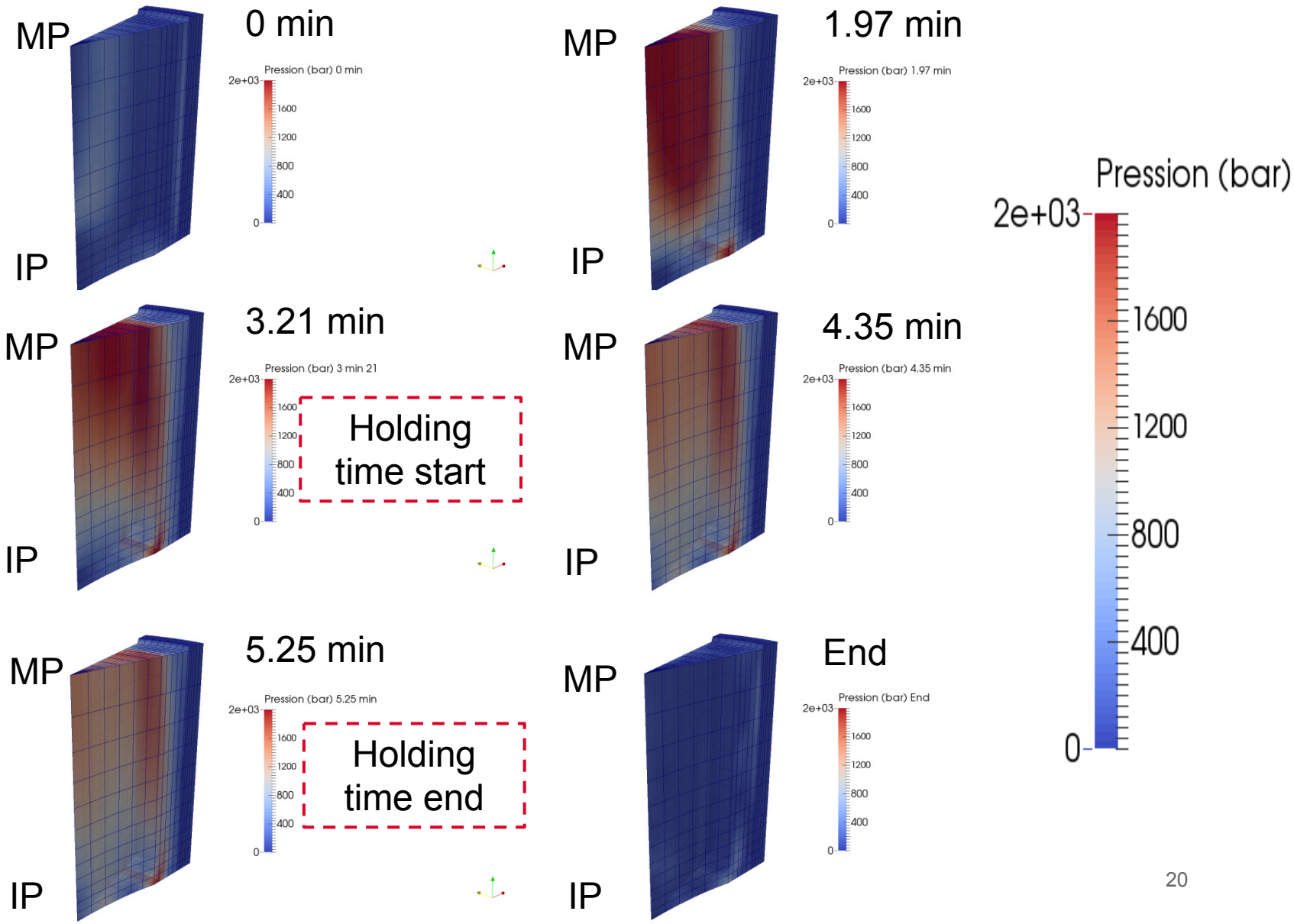
3D CALCULATIONS OF FISSION PRODUCT RELEASE

PRESSURE DISTRIBUTION IN A FUEL FRAGMENT DURING THE RAMP

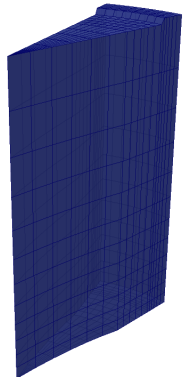
I, CS AND TE RELEASE FROM THE FRAGMENT DURING THE RAMP

LOCALISATION OF GAS RELEASE IN THE PELLET

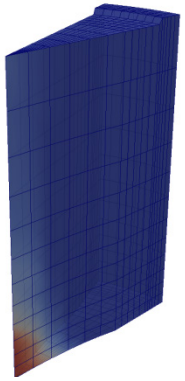
3D-PRESSURE IN A FUEL FRAGMENT DURING THE RAMP



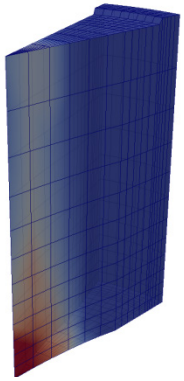
I, CS AND TE RELEASE FROM THE FRAGMENT DURING THE RAMP



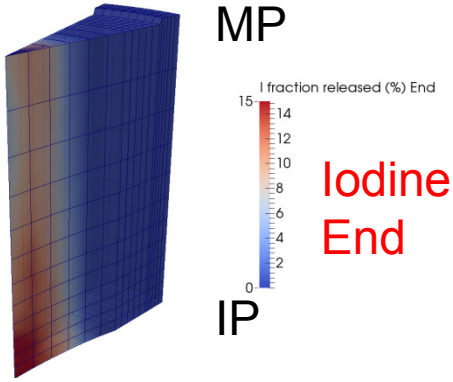
Iodine ; 0 min



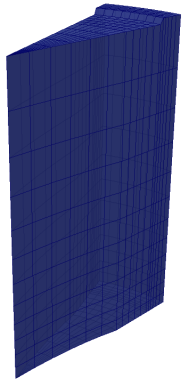
Iodine ; 3.21 min



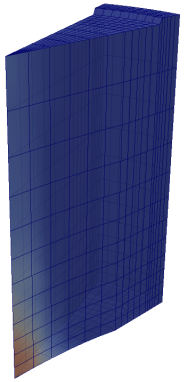
Iodine ; 5.25 min



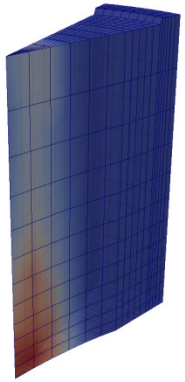
Iodine ; End



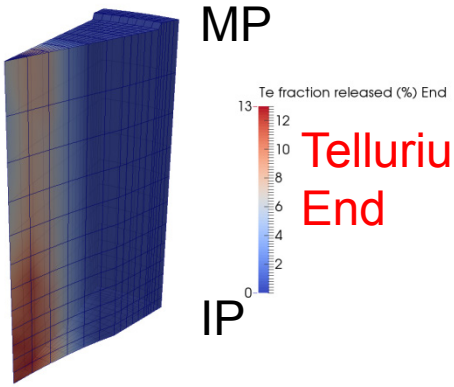
Tellurium ; 0 min



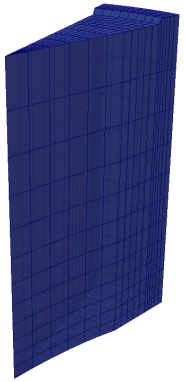
Tellurium ; 3.21 min



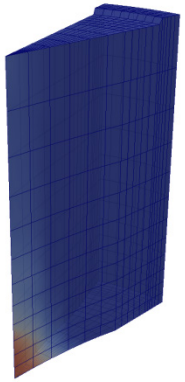
Tellurium ; 5.25 min



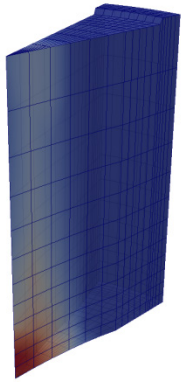
Tellurium ; End



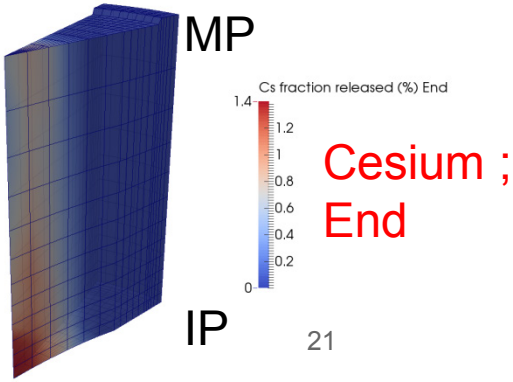
Cesium ; 0 min



Cesium ; 3.21 min



Cesium ; 5.25 min



Cesium ; End

LOCALISATION OF RELEASE IN THE PELLET

During the transient and the beginning of the holding time

- Very high pressure at the mid-pellet plane limits the release of volatile fission product in forbidding the generation of gaseous volatile compounds

- Low pressure at the inter-pellet plane **allow the volatile fission product to form gaseous compounds**, and so to be **released.**

Evolution During the holding time to the end of the calculation

- Decrease of the pressure at the mid-pellet plane allow fission products to form gaseous compounds, and so to be released

The 3D-calculation takes into account the real geometry of the pellet, leading to differencies on the time-release of volatile fission products due to axial pressure gradients in the pellet.

CONCLUSION AND PERSPECTIVES

CONCLUSION AND PERSPECTIVES

Conclusion on ALCYONE–ANGE coupling for the modelling of short holding time power ramps

- Provides good results on the chemical behavior of the fuel during a power transient by comparison with SIMS observations
- Provides fission gas release taking into account the chemical affinity of the fission products
- Gives a description of the chemical state of the fuel at each node (O/M, ΔGO_2, chemical compounds created,…)
- This description of the fuel behavior during a power transient can be useful for the prediction of I-SCC initiation in cladding
- The 3D calculation accounts for the geometry of the fuel which has a strong impact on the pressure distribution and hence on the gaseous compounds distribution in the pellet.

<u>Perspectives :</u> introduction of an oxygen redistribution model to take into account the oxygen transport with the temperature gradient.

Thank you for your attention !

Aknowledgements :
L. Desgranges for providing the SIMS results
T.N. Pham for her thermochemical calculations on the Cs-Te system
and J.C.Dumas and Nathalie Barnel (EDF) for their help in this work

LONG HOLDING TIME POWER RAMP : MODELING OF THE OXYGEN REDISTRIBUTION

Redistribution in fast reactor in normal operation

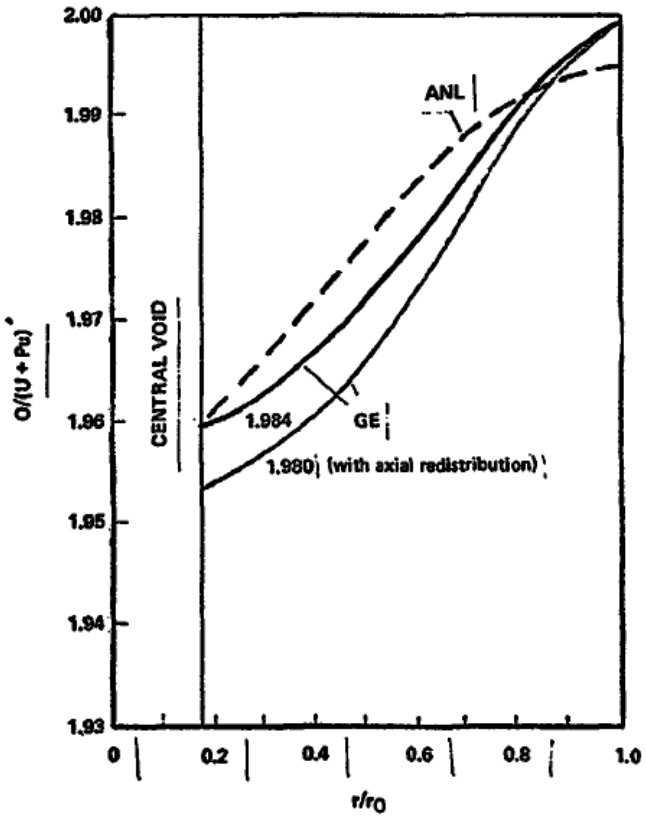
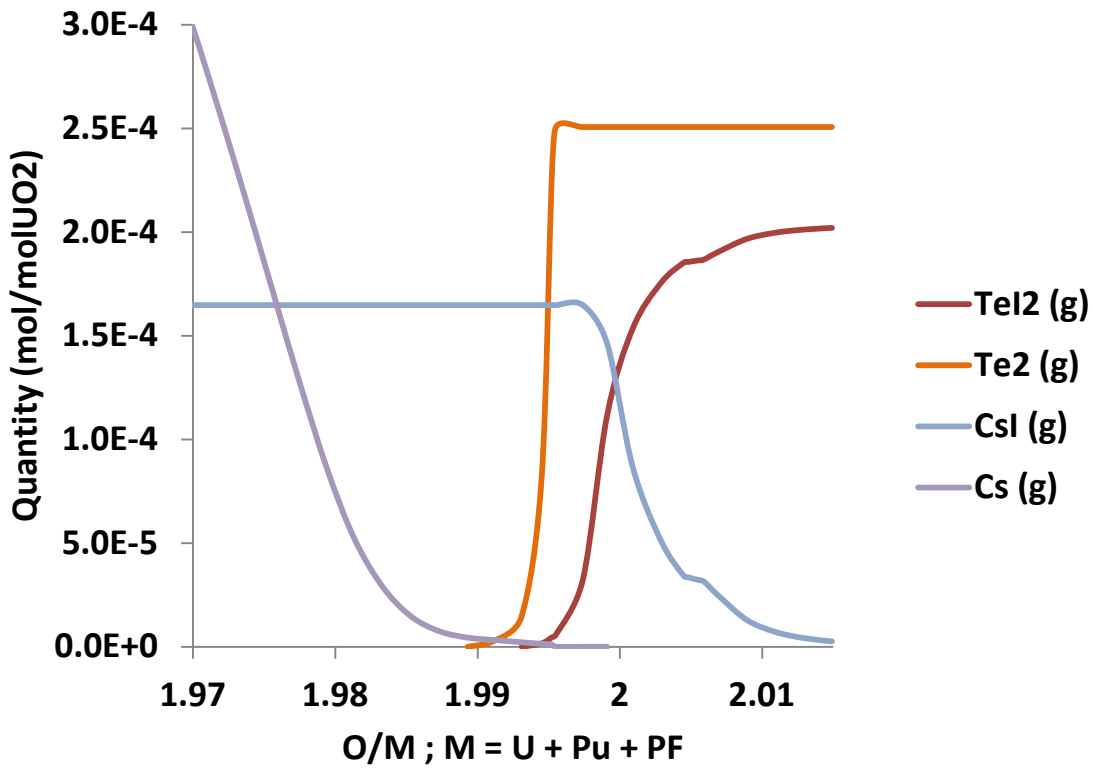


FIGURE 6. PREDICTED BEGINNING–OF–LIFE RADIAL OXYGEN–TO–METAL (O/U + Pu) PROFILES FOR P–23A TEST CASE (AVERAGE O:M = 1.984)

- In fast reactor, due to high temperature in the pellet. there is an oxygen redistribution leading to a decrease (for sub-stœchiometric fuels) of the O/M ratio in the pellet center.
- Considering O/M, M= U+Pu+PF in UO_2 irradiated fuel, with increase of Burn-Up, the fuel become more and more sub-stœchiometric.
- In power ramp, fuel temperatures through the pellet are the same as these experienced in fast reactor in normal operation.
- Oxygen quantity is an important parameter considering thermochemical equilibrium in UO_2 fuel

LONG HOLDING TIME POWER RAMP : MODELING OF THE OXYGEN REDISTRIBUTION

Consequences on the main gas in the fuel of a decrease of O/M ratio at 1800°C from ANGE calculation :



- Oxygen decrease at high temperature modify strongly the gas species available
- Considering the hypothesis made in the ALCYONE-ANGE coupling, this will have a strong impact on fission gas release.
- The OXIRED model from Lassmann is in implementation for this purpose.

K. Lassmann. JNM 150, pp 10-16, 1987

HYPOTHESIS ON FISSION PRODUCT RELEASE

- Gas release flow define by :

$$J_g = -\frac{p_g}{RT} \times \frac{k_{eff}}{\eta} \Delta P_g$$

- Release flow of a gaseous compound in minority in a gas phase :

$$J_{PF,compound} = -\frac{p_{PF,compound}}{RT} \times \frac{k_{eff}}{\eta} \Delta P_g$$

- Hypothesis : Xe release represent the majority of the release, the Pf compound are a minor part of the gas release :

$$\rightarrow J_g = -\frac{p_{Xe}}{RT} \times \frac{k_{eff}}{\eta} \Delta P_{Xe}$$

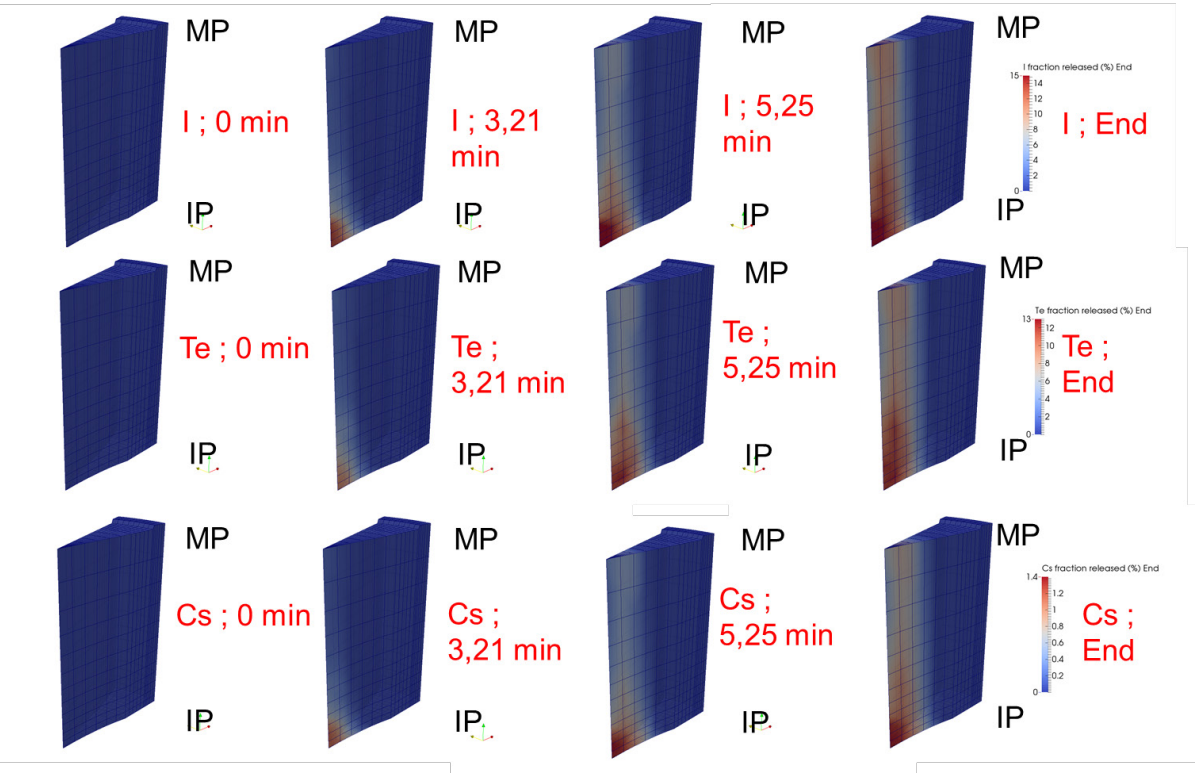
$$\rightarrow \frac{J_g}{J_{PF,compound}} = \frac{P_{Xe}}{P_{Pf,compound}} = \frac{n_{Xe}}{n_{Pf,compound}}$$

- The release quantity per second of the compound considered is given by :

$$n_{FPcompound,\,rel} = \frac{n_{FPcompound,gas\ phase}}{n_{Xe,inter\ bubbles}} \times fr_{Xe,\,rel} \times n_{Xe,tot} \ ;$$

$fr_{Xe,\ rel}$ is the Xe fraction release

LOCALISATION OF RELEASE IN THE PELLET



The very high pressure at the Mid-Pellet plane limits the release of volatile fission products during the power transient.

At the inter-pellet plane, the pressure is lower during the transient and at the beginning of the holding time, allowing the volatile fission products to be released

Then the release increases at the mid-pellet plane with the decrease of the pressure.

The 3D-calculation takes into account the real geometry of the pellet, leading to differencies on the time-release of volatile fission products due to axial pressure gradients in the pellet.