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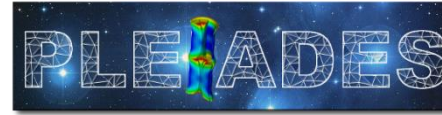
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# MODELING VOLATILE FISSION PRODUCTS TRANSPORT INTO THE GERMINAL V2 FUEL PERFORMANCE CODE BY COUPLING TO THERMOCHEMICAL SOFTWARE

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14-18 October 2018 – Seattle, WA - USA

## 1/ Context

- Integration of thermochemical component into the PLEIADES simulation platform
- Chemical state of fission products in FBR (U,Pu)O<sub>2</sub> fuel
- Specific interest for GERMINAL: JOG and FCCI description

## 2/ Thermochemistry:

- Tools: ANGE (AdvaNced Gibbs Energy minimizer) and OpenCalphad (OC)
- Models + databases: TBASE and TAF-ID

## 3/ Coupling ANGE / OpenCalphad to GERMINAL V2

- Calculation scheme
- JOG evolution with time /burnup
- Volatile FPs radial distribution
- Oxygen radial redistribution

## 4/ Next steps

- Incorporation of the cladding material constituents Cr, Fe and Ni
- Oxygen quantity available for reacting into the gap

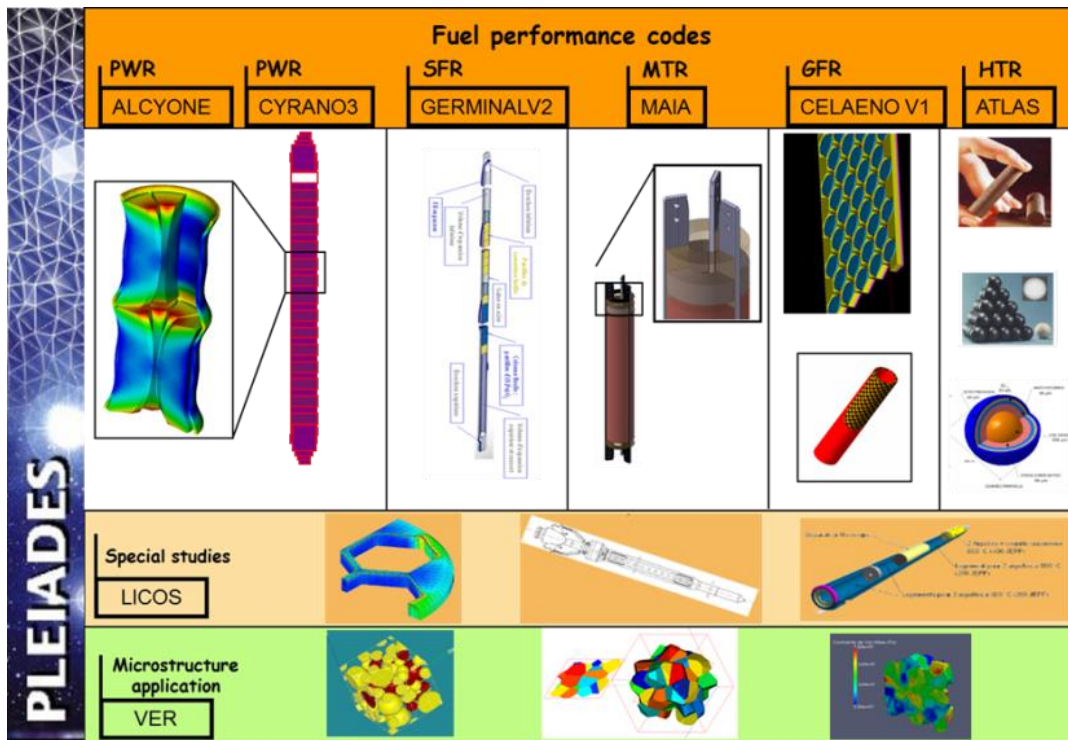
# Context: the PLEIADES fuel simulation platform – the GERMINAL code

## R&D activities in support of ASTRID (French SFR prototype project)

→ Need to update the fuel performance code for the design studies

With a validated modelling and calculation scheme for normal and off-normal conditions

→ Development of **GERMINAL V2** within **PLEIADES** simulation framework



- Multi-physic fuel coupling  
⇒ taking into account the thermochemistry is needed in order to describe exp. observations performed during power transient

### ☞ Main goals:

- PWR: to simulate the cladding failure by SCI (Stress Induced Corrosion)
- SFR: to be representative of the chemical state of the FPs in our description of the JOG formation and of the FCCI

## PLEIADES: Federative framework for fuel performance codes

Co-developed by CEA, EDF and FRAMATOME

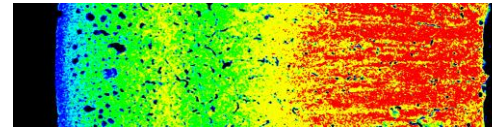
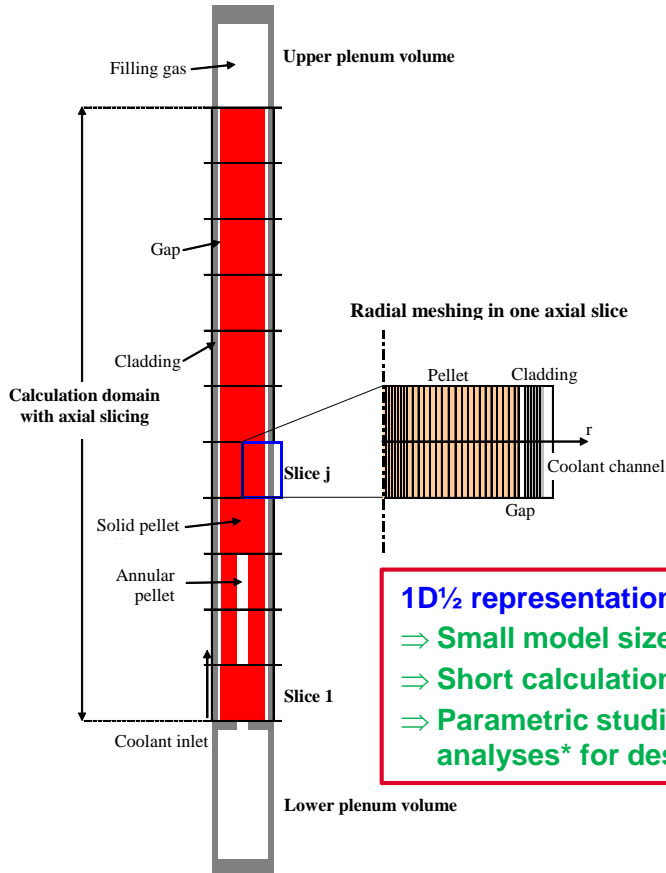
# General presentation of GERMINAL

## 1D $\frac{1}{2}$ calculation scheme

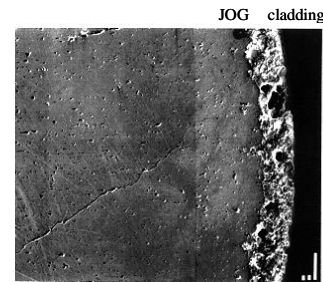
- Geometry assimilated to a **revolution cylinder**
- Fuel pin decomposed into **axial slices**  
Thermal evolutions linked by heat removal by coolant
- **Radial resolution** of coupled physical processes **in each axial slice**  
Thermal analysis, mechanics, fuel physics & chemistry

## Special features of SFR fuel pins

- High temperature conditions:  
  - ≈ 2200°C at pellet center, 1000°C at periphery
  - High temperature gradients : ≈ 5000°C / cm
- Radial migration of elements (O, U, Pu)
- Radial migration of porosity (central hole formation)
- Preponderant gas release (80-90% at end-of-life)
- Volatile FPs release → "Joint Oxyde-Gaine" formation
- Steel material for cladding ; important damage & swelling



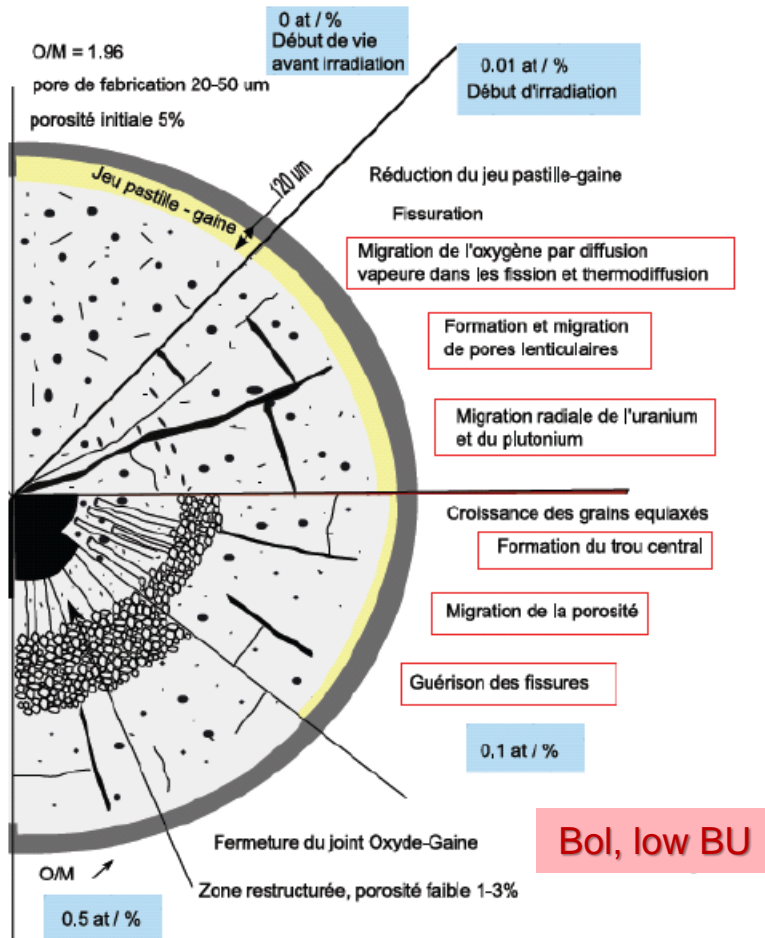
Colored X picture  
Pu redistribution



PHENIX pellet, initially solid  
Final burn-up : 13,3 at%

## FBR fuel behaviour

Very high thermal level  $\Rightarrow$  enhanced phenomena



## Current description (into GERMINAL V2) :

$\rightarrow$  Relatively empirical, deduced from qualitative PIE performed into the Phénix Reactor (in the 80's)

$\Leftrightarrow$  based on the similarity between the cesium and the (stable) fission gases retention

### For the JOG : $\text{JOG} = \text{porous } \text{Cs}_2\text{MoO}_4$

✓  $\lambda(\text{JOG}) = f[\lambda(\text{Cs}_2\text{MoO}_4), p(\text{JOG})]$  for low porosity

✓  $= f[\lambda(\text{Cs}_2\text{MoO}_4), \lambda(\text{gas}), p(\text{JOG})]$  for high porosity

### The ROG (FCCI) :

✓  $\frac{\partial e_{\text{corr}}}{\partial \tau} = +10 \mu\text{m/at}\%$  undeformed cladding

✓  $\frac{\partial e_{\text{corr}}}{\partial \tau} = +15 \mu\text{m/at}\%$  deformed cladding

## Limitations:

Real chemical composition of the JOG, more complex, is not considered

Thermodynamic of the fuel is not considered (oxygen chemical potential -  $T^\circ$ ,  $p(\text{O}_2)$ , FPs activities, presence of liquid phases)

$\Rightarrow$  Goal  $\Rightarrow$  to develop a description of the JOG + ROG on physical basis (namely thermodynamic + transport)



# Chemical state of fission products in irradiated oxide fuel

✓ Each fission creates 2 FPs:

IA		IIA												IIIB		IVB		VB		VIB		VIIB		VIII									
H		Gas and Volatiles												Metallic precipitates																He			
Li	Be	Oxides precipitated												Oxides in solution																			
Na	Mg	IIIA	IVA	VA	VIA	VIIA	VIII					IB	II B	Al	Si	P	S	Cl	Ar														
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr																
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe																
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn																
Fr	Ra	Ac																															
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu																	
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr																	

⇒ Modification of physical and chemical properties of the irradiated material: thermal conductivity, creep, grain size, fission gas release...

☞ The chemical state of the fuel depends strongly of the oxygen chemical potential of the solid solution  $(U_{1-y}Pu_y)O_{2-x}$  :

$$\Delta G_{O_2}(x, y, T) = \mu(O_2) = RT \ln(p_{O_2}/p^\circ_{O_2})$$

- R: Perfect Gases Constant (8.314J/mol/K)
- T: Temperature (K)
- $P(O_2)$ : oxygen partial pressure (bar)
- $P^\circ(O_2)$ : standard pressure (1 bar)

	Element	Yield (% PF/fission)	Total (% / fission)
PF in solid solution	Y	1.9	45
	La	5.6	
	Ce	11.4	
	Pr	4.8	
	Nd	15.5	
	Pm	1.2	
	Sm	3.4	
	Eu	0.6	
	Gd	0.4	
	Rb	1.5	
Cs	20.1		
Sr	3.6		
Ba	6.8		
Zr	19.2		
PFs forming oxide precipitates	Nb	0.2	75
	Mo	21.3	
	Tc	5.5	
	Ru	22.0	
	Rh	5.8	
	Pd	13.8	
	Ag	1.3	
	Cd	1.0	
	In	0.1	
	Sn	0.5	
	Sb	0.2	
	Te	3.5	
Gases and volatile FPs	He	0.8	28
	Kr	1.8	
	Xe	23.6	
	Br	0.1	
	I	1.7	

Fission products creation in a Phénix fuel pin at 10 %FIMA

# Thermochemical components available in PLEIADES: ANGE and OC\* (OpenCalphad)

## ■ Open source thermodynamic softwares:

- ANGE : AdvaNced Gibbs Energy minimizer, SOLGASMIX based code which has been implemented into the PLEIADES fuel simulation platform (partnership CEA and EDF)
- OC: OpenCalphad, developed by Bo Sundman (formerly KTH - INSTN), one of the first developer of the Thermo-Calc software


## ■ Principle:

→ Calculation at fixed T and P or V of the thermochemical equilibria of the different chemical constituents located in the different (solid, liquid and gaseous) phases, under the species balance constraint by **minimising the free enthalpy** (or **Gibbs free energy**) of the whole system.

## ■ Thermodynamic models for the mixture phases:

- *Lindemer & Besmann description* for the  $(U,Pu,PF)O_{2-x}$  solid solution in ANGE: neutral compounds with a given cation valency
- CEF (*Compound Energy Formalism*) with OC
  - CEF based on the CALPHAD method with several sub lattices (anionic, cationic, with vacancies)
  - ⇒ In order to reproduce the stoichiometry of the phases considered

## ■ Thermodynamic databases:

- (TBASE + SGTE) with ANGE 
- (TAF-ID) with OpenCalphad 

\* B. Sundmann, U.R. Kattner, M. Palumbo and S.G. Fries  
"OpenCalphad - a free thermodynamic software"  
*Integrating Materials and Manufacturing Innovation*, 4:1 (2015)

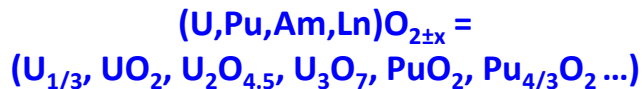


# Comparison of the thermodynamic databases

## ■ ANGE

### ☞ TBASE + Lindemer & Besmann's model

- Database from the 90's with regular thermodynamic functions updating
- 24 elements of the periodic table
- Lindemer & Besmann's description (associated species model) for the mixed oxide
- ➔ (sub-)regular solution of:

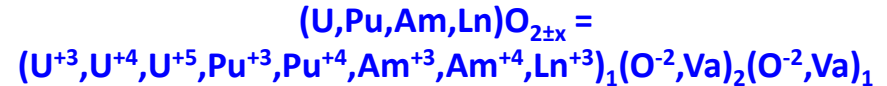


- *Stoichiometric compounds (100)*
- *Metallic precipitates description quite simplist: only one phase of « noble metals »*
- ➔ Quite simple models that do not describe the non-stoichiometry of the phases as well as the liquid solutions

## ■ TAFID\_V8 (beginning 2018)

### ☞ CEF + Thermo-Calc or OC (Open Calphad)

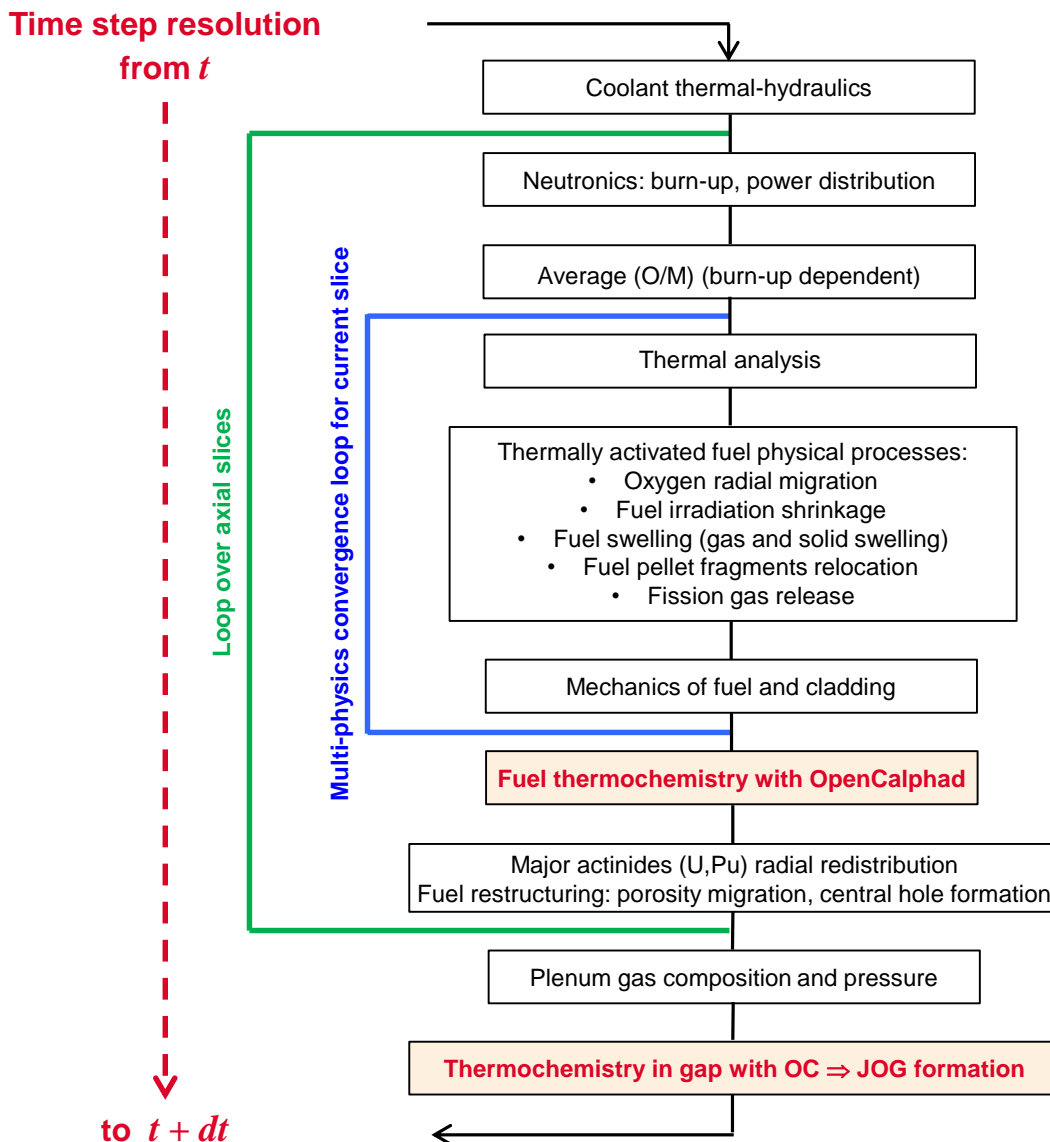
- Database developped and maintained in the frame of the TAF-ID project (OECD/NEA)
- 41 elements of the periodic table
- Model CEF ⇔ *sub-lattice description in relation with crystalline structure for the mixte oxide*
- ➔ non ideal solution of:



- *Phases stoichiometry range (~ 150) described*
- *Description of the mixture liquid phases, including the various metallic precipitated phases*
- ➔ Complete model describing the non stoichiometry of the phases as well as the formation of liquid solutions

- ☞ More phases as well as more sophisticated models implemented into the TAF-ID
- ➔ More representative of the phase transitions and of cristallographic defects
- ➔ but still in test and validation state

## Coupling GERMINAL with a thermochemistry component



- Thermodynamic equilibrium calculation in the fuel pellet after local convergence loop

$\Leftrightarrow$  System with 16 elements:

He, U, Pu, O, Cs, Te, I, Mo, Ba, Zr, Ce, La, Gd, Eu, Ru, Pd

$\rightarrow$  Quantities of gaseous and liquid volatile fission products phases released into the gap

- Fission products release: 4 options

✓ **Options 1 and 2:** Total release of VFPs gaseous / (gaseous + liquid) phases formed into a radial mesh directly into the fuel-to-clad gap

✓ **Options 3 and 4:** Release of VFPs gaseous/ (gaseous + liquid) phases homothetic to stable gases release

- Thermodynamic equilibrium calculation in the gap  $\Leftrightarrow$  System with 6 or 7 elements :

Cs, Te, I, Mo, Ba, Zr, Pd, O

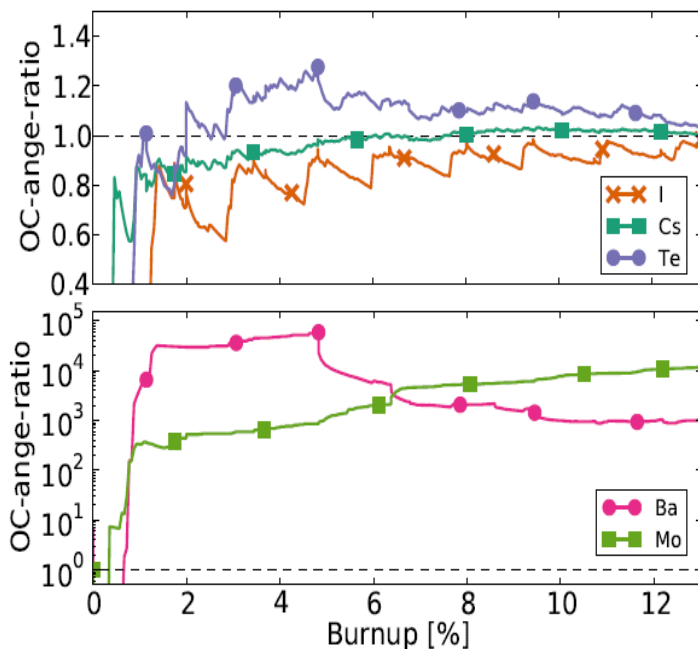
$\rightarrow$  Nature and quantities of solid and liquid phases contributing to the JOG formation

### Difficulties

- Convergence of thermodynamic equilibrium
- Calculation times

# Résultats GV2-ANGE / OpenCalphad : Composition chimique de la pastille combustible

- Chemical composition of the JOG calculated at  $T^\circ(\text{gap})$  :
  - With ANGE : Cs + CsI +  $\text{Cs}_2\text{Te}$  calculated in the gap in irradiation conditions
  - With OpenCalphad : Mo + BaO + liquid (Cs,I,Te,O,Mo)
- Chemical composition of the JOG calculated at room  $T^\circ \Leftrightarrow$  PIE conditions
  - With ANGE : phases identical to those obtained at  $T^\circ(\text{irr})$  ;  
low  $\text{Cs}_2\text{MoO}_4$  content
  - With OpenCalphad : Mo + Cs + CsI +  $\text{Cs}_2\text{Te}$  + BaO +  $\text{Cs}_2\text{MoO}_4$



Hadix-1 : 3,8 %FIMA

BCC_A2(CS)	2,6800E-4
CS2TE	2,1962E-4
CSI_B2	6,7640E-5
BA2ZRO4	4,8E-13
BCC_A2(MO)	3,5130E-5
HALITE (BAO)	1,0943E-5
CS2MOO4_S1	1,3761E-5

Nestor-3 : 13,3 %FIMA

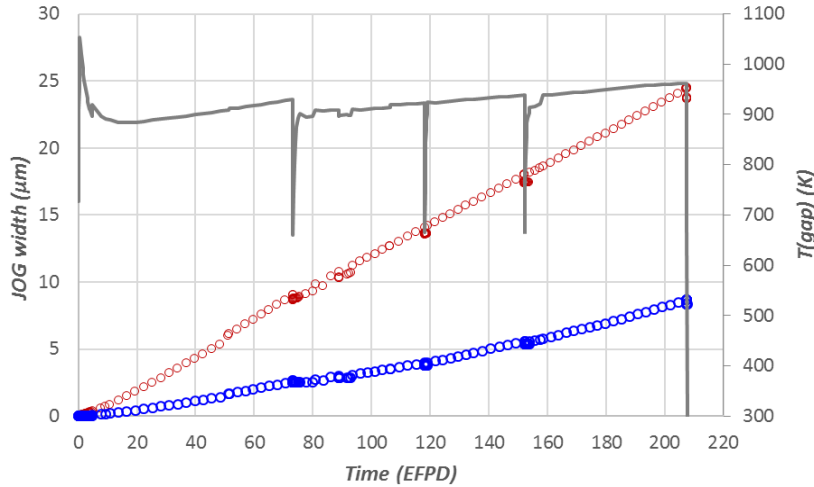
BCC_A2(CS)	4,246E-4
CS2TE	1,0391E-3
CSI_B2	3,291E-4
BA2ZRO4	3,90E-12
BCC_A2(MO)	2,379E-4
HALITE (BAO)	5,390E-5
CS2MOO4_S1	2,1941E-3

✓ Evolution versus burnup of the ratio of volatile FPS release between OC and ANGE:

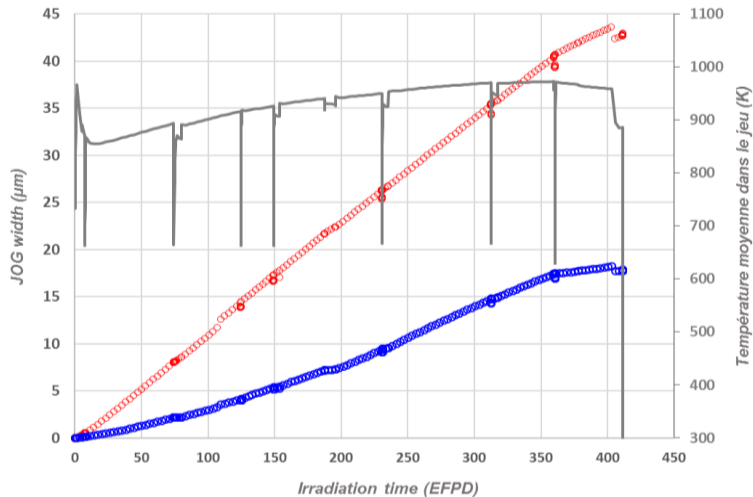
- Similar values for Cs, Te and I
- Ba and Mo are not predicted similarly with GERMINAL + ANGE vs GERMINAL + OC: thermodynamic database specificities

# Results GERMINAL V2 - ANGE: Evolution of JOG width ( $\mu\text{m}$ ) versus time

Exp. Hadix-1 : 3,8 %FIMA



BOITIX1 - 7,0 %FIMA -  $e(\text{JOG}) = f(t)$

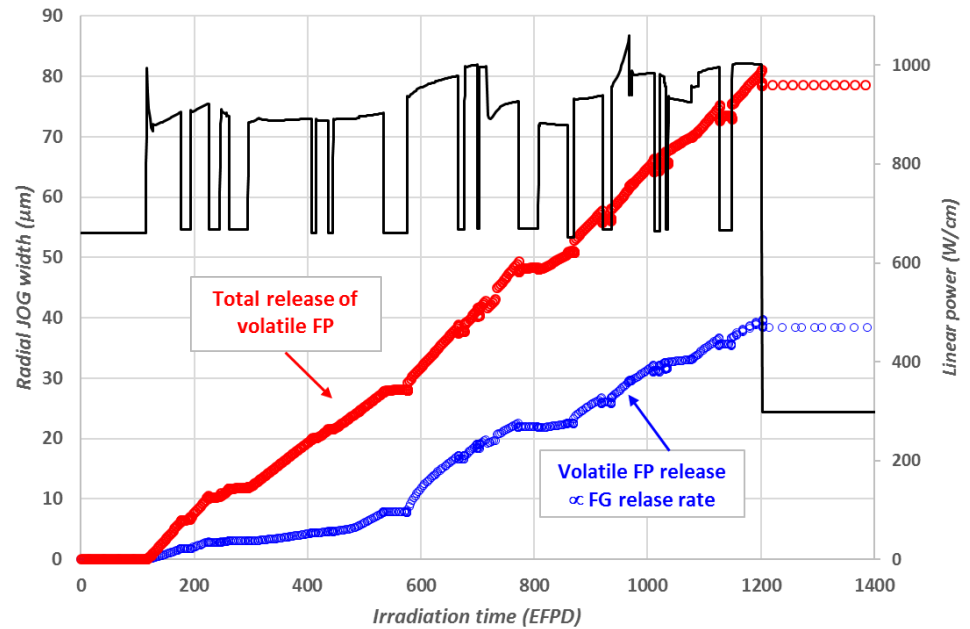


Principe : from  $n_i(\varphi_i)$

$$e(\text{JOG}) = \sum e(\varphi_i) = \sum n_i(\varphi_i) \times \frac{Vm(\varphi_i)}{2\pi R_{ext} \text{ comb}}$$

with  $Vm(\varphi_i) = \frac{n(\varphi_i)}{\rho(\varphi_i)}$  : molar volum of the  $i$ th phase

NESTOR-3 experiment (13,3 %FIMA) : evolution of the JOG width versus time calculated with GERMINAL V2 + ANGE



- Scheme operationnal with ANGE
- With OC: calculation is performed a posteriori in autonomous mode from the gap inventory

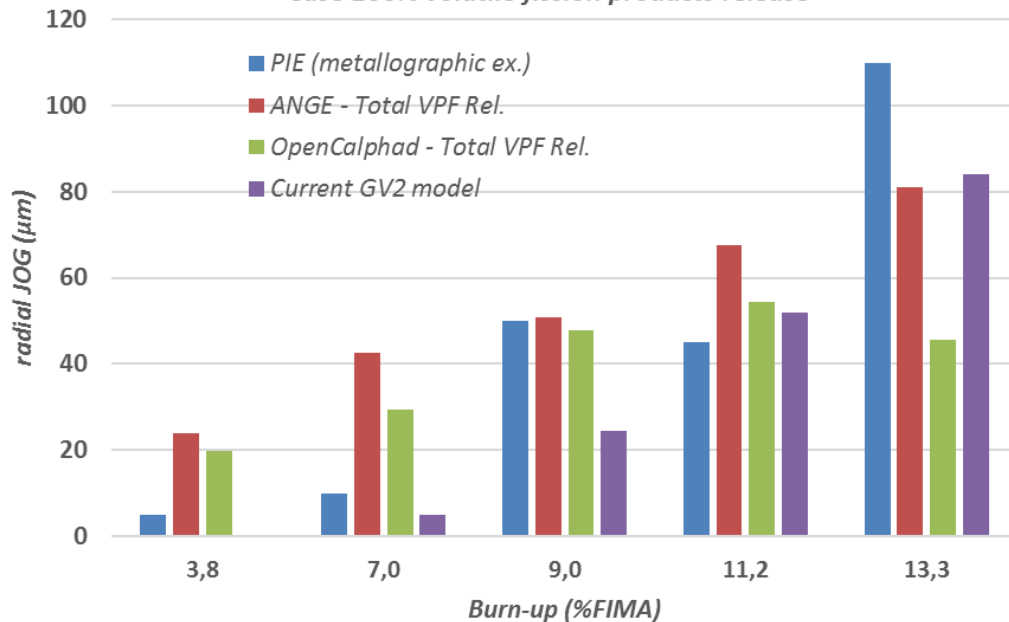
# RESULTS GERMINAL V2-ANGE / OC : JOG WIDTH VERSUS BURN-UP (1)

- Final JOG widths calculated at T = 298.15K (room temperature ⇔ PIE) at the PPN (Peak Power Node = maximum flux) for following experiments:

HADIX-1 , BOITIX-1, COUCOU-1, SPHINX-1, NESTOR-3 :  
| 3,8 %FIMA | 7,0 %FIMA | 9,0 %FIMA | 11,2 %FIMA | 13,3 %FIMA |

## Case 100% VFP (volatile fission products) release

JOG width versus final Burn-up:  
Case 100% volatile fission products release



VFP Rel. = 100%	HADIX-1	BOITIX-1	COUCOU-1	SPHINX-1	NESTOR-3
Burn-up (%FIMA)	3,8	7,0	9,0	11,1	13,3
e(JOG) - Exp (µm)	5	10	50	45	110
e(JOG) - ANGE (µm)	24	43	51	67	81
e(JOG) - OC (µm)	20	29	48	55	46
e(JOG) - GV2 (µm)	0	5	25	52	84

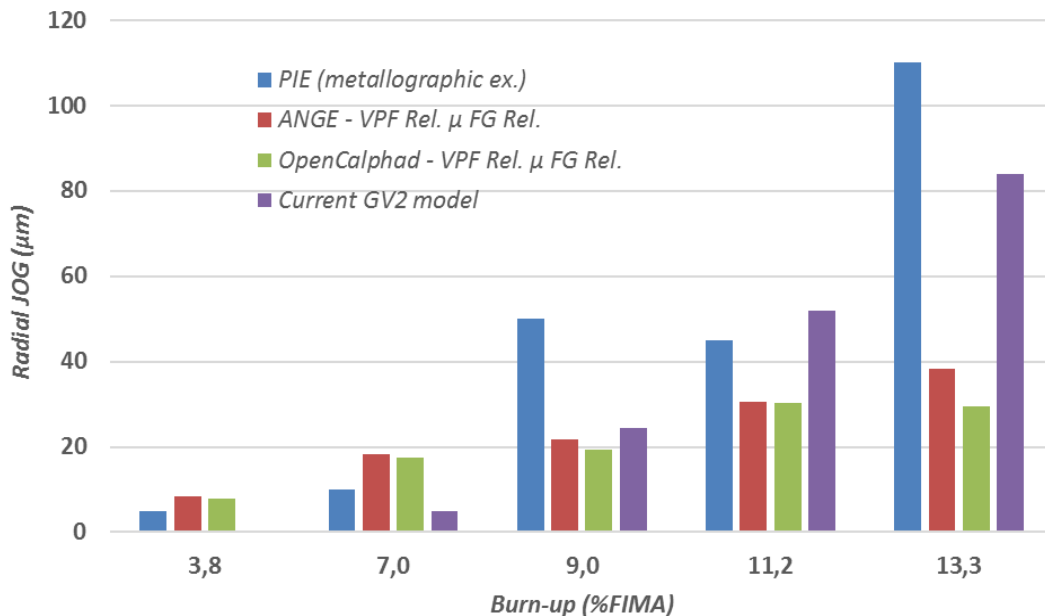
# RESULTS GERMINAL V2-ANGE / OC : JOG WIDTH VERSUS BURN-UP (2)

- Final JOG widths calculated at T = 298.15K (room temperature ⇔ PIE) at the PPN (Peak Power Node = maximum flux) for following experiments:

HADIX-1 , BOITIX-1, COUCOU-1, SPHINX-1, NESTOR-3 :  
| 3,8 %FIMA | 7,0 %FIMA | 9,0 %FIMA | 11,2 %FIMA | 13,3 %FIMA |

Case: VFP release ∝ FG  
(fission gas) release

JOG width versus final Burn-up:  
Volatile fission products release ∝ Fission gas release



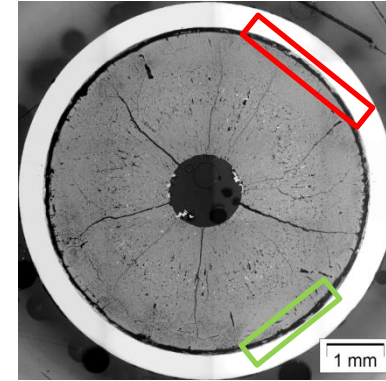
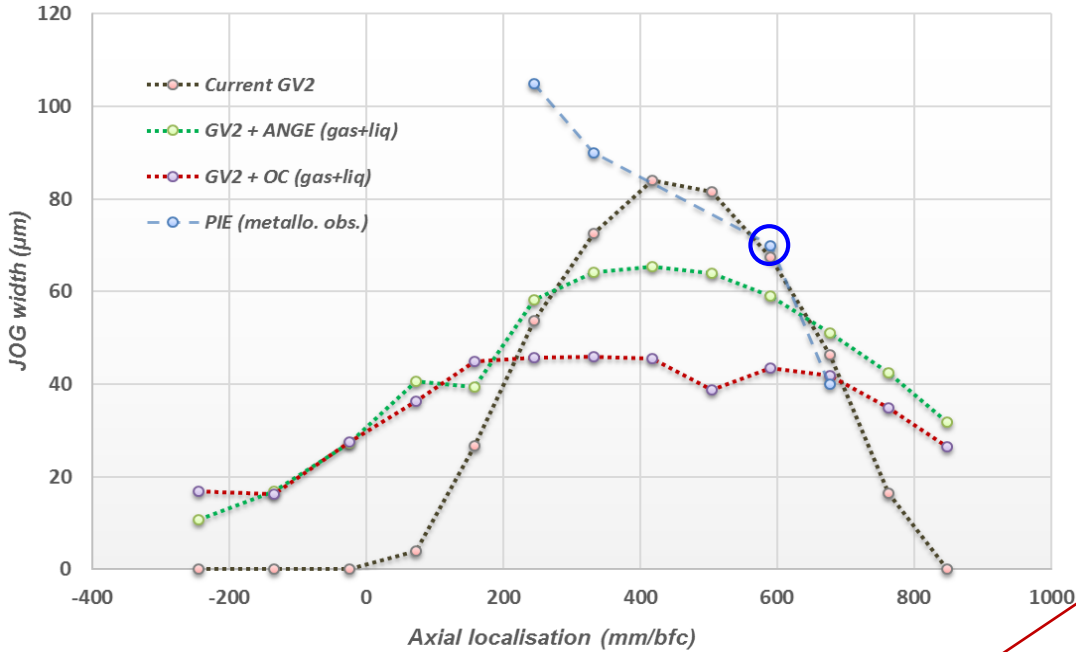
VFP Rel ∝ FG Rel.	HADIX-1	BOITIX-1	COUCOU-1	SPHINX-1	NESTOR-3
Burn-up (%FIMA)	3,8	7,0	9,0	11,2	13,3
e(JOG) - Exp (µm)	5	10	50	45	110
e(JOG) - ANGE (µm)	8	18	21	30	38
e(JOG) - OC (µm)	8	17	19	30	29
e(JOG) - GV2 (µm)	0	5	25	52	84



# CALCULATION NESTOR-3 GV2-ANGE / OC: JOG WIDTH VERSUS AXIAL POSITION

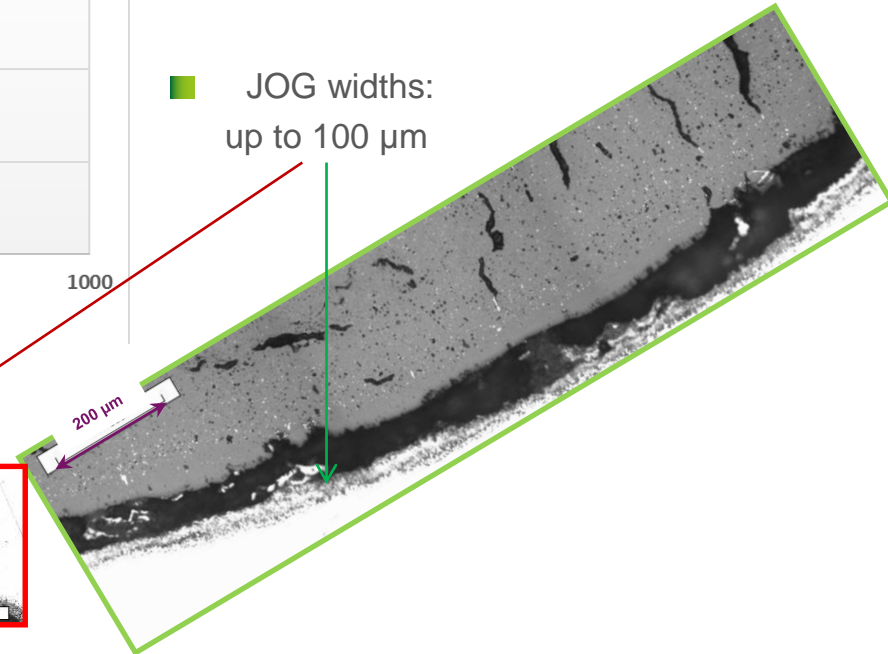
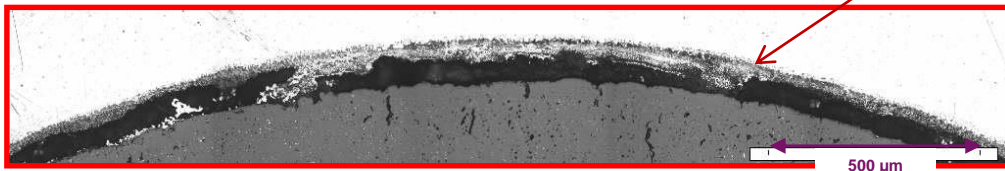
NESTOR-3 exp. -  $(U_{0.78}Pu_{0.22})O_{1.975}$  -13,3 %FIMA

$(U_{0.78}Pu_{0.22})O_{1.975}$  irr. up to 13,3 %FIMA:  
Axial JOG evolution (at the end of irradiation)



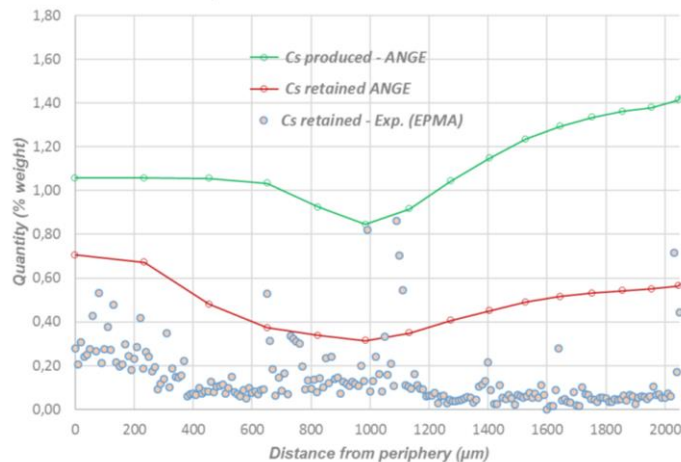
1400 mm

JOG widths:  
up to 100 µm

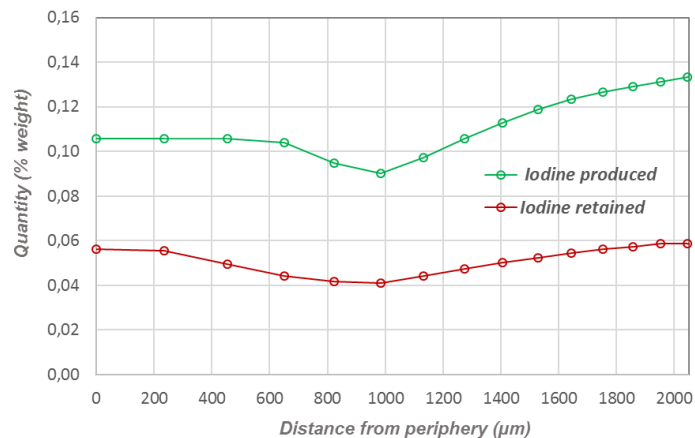


# Comparison GERMINAL V2 - ANGE /OpenCalphad: Radial distribution of Volatile Fission Products

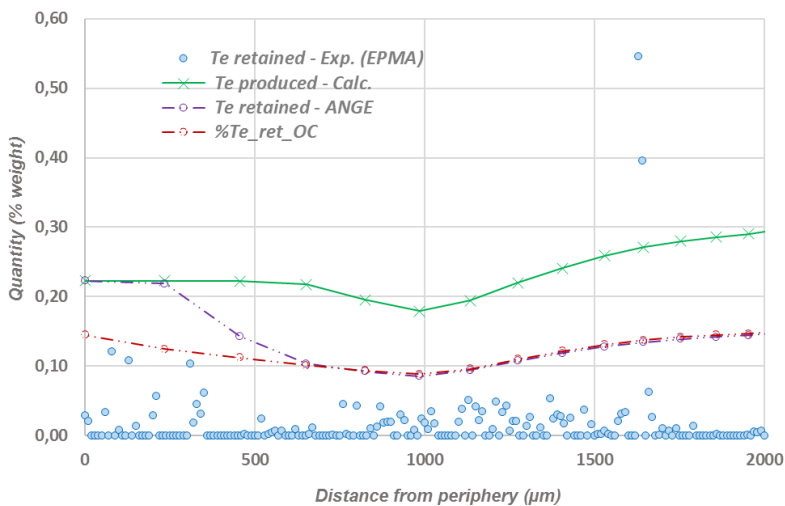
NESTOR-3 - 13.3 %FIMA :Radial distribution of cesium at PPN and at eol calculated by GERMINAL + ANGE - Case VFP release  $\propto$  FG release



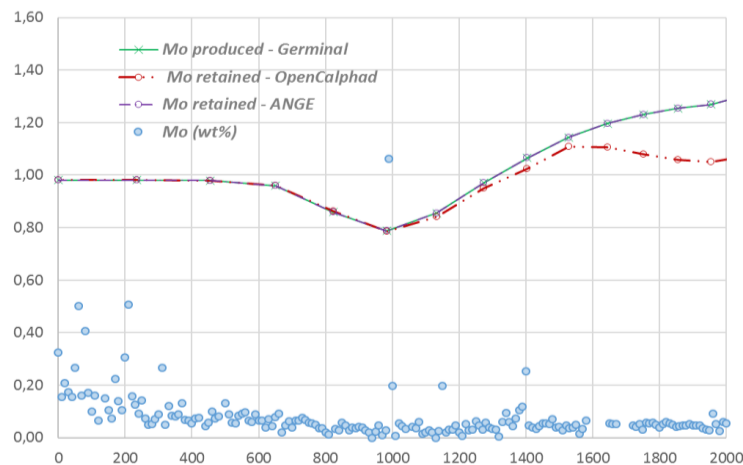
NESTOR-3 - 13.3 %FIMA :Radial distribution of iodine at PPN and at eol calculated by GERMINAL + ANGE - Case VFP release  $\propto$  FG release



NESTOR-3 - 13.3 %FIMA :Radial distribution of cesium at PPN and at eol calculated by GERMINAL + ANGE - Case VFP release  $\propto$  FG release

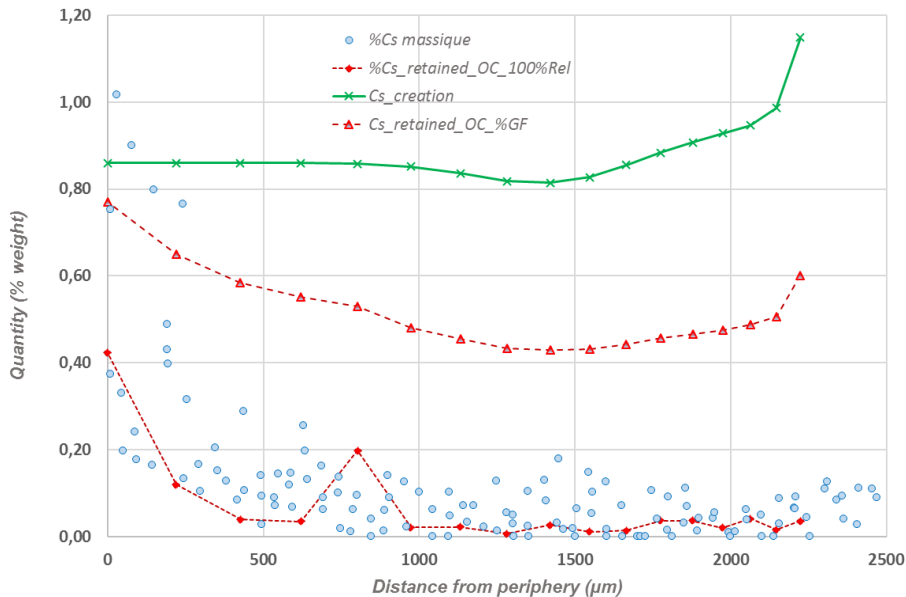


NESTOR-3 - 13.3 %FIMA :Radial distribution of molybdenum at PPN and at eol calculated by GERMINAL + ANGE - Case VFP release  $\propto$  FG release

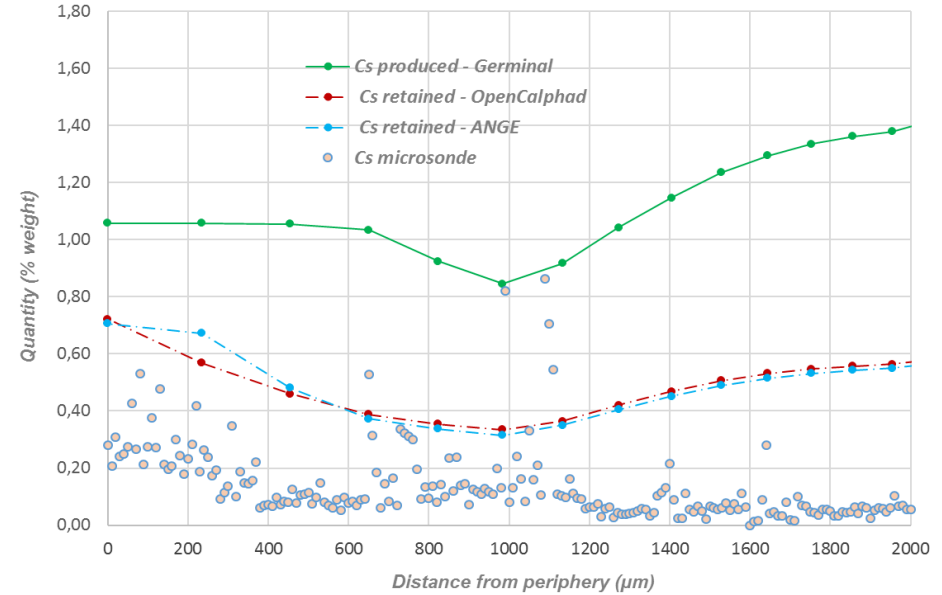


# Calculation GERMINAL V2 - OpenCalphad: Cesium radial distribution

Coucou1 - 9,0 %FIMA - Cesium radial evolution



NESTOR-3 - 13.3 %FIMA :Radial distribution of cesium at PPN and at eol  
calculated by GERMINAL + ANGE - Case VFP release  $\propto$  FG release



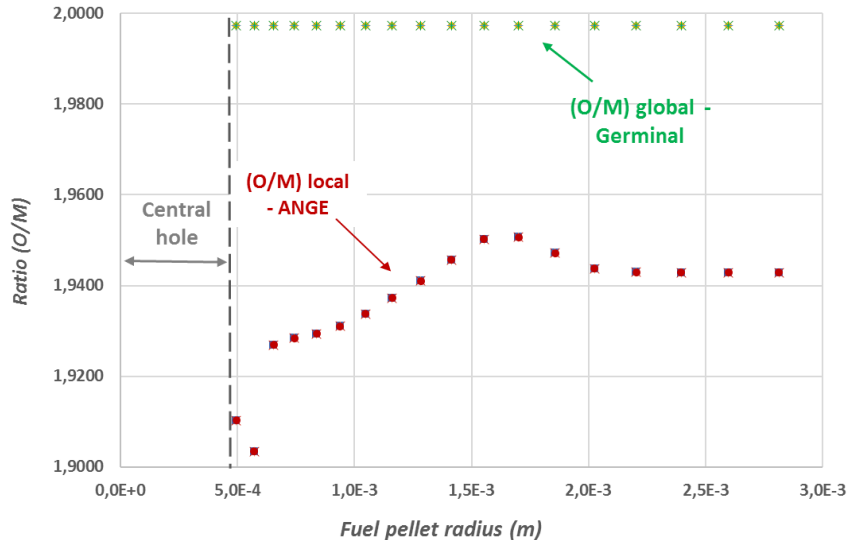
☞ Results seem to be more consistent when we consider only partial (an not total) release of VFP = volatile fission products

# O/M ratio evolution with burnup: Results GERMINAL V2 - ANGE

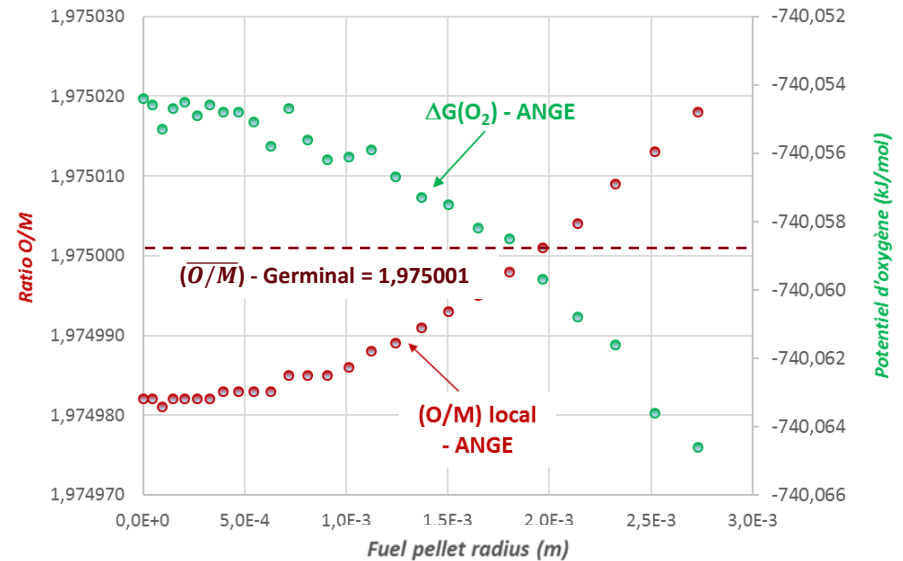
Hadix1 - 3,8 %FIMA -  
PPN - 207,6 EFPD

Nestor3 - 13,3 %FIMA -  
PPN - 56,5 EFPD

HADIX1 - 3.8 %FIMA - VPF ReL.  $\propto$  FG Rel. - end irr. 207,6 EFPD



Nestor3 - 56,5 JEPP - Cas 100% Relâch. PF volatils



⇒ Local O/M ratio in the fuel pellet:

Difference between Germinal law and thermochemistry evaluation with ANGE irradiation goes up with time..

# Conclusion - Outlooks

## ■ Inventory JOG-ROG:

- Taking into account palladium (Pd) as volatile FP in the calculation procedure:
  - can be found in metallic inclusions with Te (and Ag) on liquid state from the low temperatures ( $\sim 700$  K)
- taking into account constituents of the cladding material Fe, Cr and Ni:
  - chemical composition of ROG phases to come
  - volatile FPs release law: description more phenomenological to develop

## ■ Oxygen key-role:

- Coupling with the oxygen radial redistribution model:
  - taking into account the average  $(\overline{O/M})_{\text{slice}}$  ratio given by the thermochemistry as an input for the OXIREM model in order to have the radial redistributed  $(\overline{O/M})_{\text{local}}$  ratio
    - to introduce into the coupling with OpenCalphad
- Work /study on the oxygen available into the gap:
  - Influence of the available oxygen on chemical equilibria:
    - oxygen in excess in the fuel-to-clad gap ?
    - oxygen in excess on the fuel pellet surface ?
    - Taking into account the oxygen activity instead of the oxygen quantity?

Complementary slides



## Thermochemical component ANGE (*AdvaNced Gibbs Energy minimizer*)

⇔ SAGE (*SOLGASMIX Advanced Gibbs Energy*)

### Thermodynamic database + models:

Gaseous Phase	Ideal Mixture (IDMX = « <i>Ideal Mixture</i> »)
(U,Pu,L*)O <sub>2-x</sub> : Fluorite matrix in solution with its FPs (L* = Lanthanides)	Sub-regular solution (RKMP = <i>Redlich Kister Muggianu Polynomial</i> )
Metallic precipitates	Ideal mixture (IDMX)
Separated compounds (stoichiometric solid /liquid phases)	$\Delta G_f^\circ(T) = A + B \times T$ (Standard formation energy - J/mol)

### PWR database:

22 elements  
61 gaseous compounds  
80 stoichiometric compounds  
3 compounds for metallic precipitates  
19 species in solid solution (U,Pu,L\*)O<sub>2-x</sub> (L\* = Lanthanides)

### SFR database:

24 elements  
90 gaseous compounds  
100 stoichiometric compounds  
5 compounds for metallic precipitates  
27 species in solid solution (U,Pu,L\*)O<sub>2-x</sub>

### FPs in solution modeling:

⇒ Lindemer & Besmann (L&B) description:

- <U<sub>1-y</sub>Pu<sub>y</sub>O<sub>2-x</sub>> irradiated = (U,Pu,L\*)O<sub>2-x</sub>: avec L\* = Gd, La, Nd.. mixture of chemical species PuO<sub>2</sub>, Pu<sub>4/3</sub>O<sub>2</sub>, UO<sub>2</sub> et U<sub>2</sub>O<sub>4.5</sub> (or U<sub>3</sub>O<sub>7</sub>), UL\*<sub>2</sub>O<sub>6</sub> and L\*<sub>4/3</sub>O<sub>2</sub> representative of the valency state
- Description semi-empirical not representative of cristallographic defects



# TAF-ID Project (OECD/NEA) : Thermodynamic Advanced Fuels-International Database

## TAF-ID V8 database (2018) :

- 41 elements :
- ~ 200 binary systems
- ~ 75 ternary systems

Introduction of models for binary and ternary systems

### TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home Introduction Models Phases **Systems**

Elements  
Assessed binary systems  
Assessed ternary systems  
Systems with Ag, Al, Am, Ar, B, Ba, C, Ca, Ce, Cr, Cs, Fe, Gd, H, He, I, La, Mg, Mo, N, Nb, Nd, Ni, Np, O, Pd, Pu, Re, Rh, Ru, Si, Sr, Ta, Tc, Te, Th, Ti, U, V, W, Zr  
Periodic table

### TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home Introduction Models Phases **Systems** TDB

**Introduction**  
**Thermodynamic models**  
**Phases described**  
usual name  
database name  
prototype  
StrukturBericht table  
**Assessed systems**  
elements  
binary systems  
ternary systems  
periodic table

To support the development of Generation 4 reactors (SFR, SCWR, GFR, LFR, MSR, VHTR) and to contribute to lifetime extension, safety improvement and safety analysis for Generation 2 & 3 systems (PWR, BWR, PHWR), there is a need to make available a comprehensive, internationally recognized, and quality-assured thermodynamic database. For this reason, a joint Project between 9 organizations representing 6 member states coordinated by the OECD-Nuclear Energy Agency (NEA) was started in 2013 with an Initial 3 years period. The objective of the project titled Thermodynamics of Advanced Fuels - International Database (TAF-ID) is to develop a thermodynamic database using the Calphad method to perform thermodynamic calculations on different types of fuels (oxide, metallic, nitride, carbide) including minor actinides (Am, Np), fission products (Cs, I, Ba, Sr, Mo, Zr, lanthanides, metallic fission products) and structural materials (steel, Zr alloy, B4C, SiC, concrete). Thermodynamic properties of fuels versus temperature and composition (with fission products and minor actinides) will be provided. The inclusion of structural materials will allow the prediction of fuel/cladding chemical interactions under normal and off-normal conditions. The database will be generated and regularly updated by merging existing and developing databases from the various participating organizations. The database will be available in both Thermo-Calc and FACTSAGE usable formats.

**Members of the Programme Review Group:**

Country	Signatory	Representative	Alternate member
Canada	AECL, RMCC, UOIT	M. Piro	E.C. Corcoran
France	CEA	C. Guéneau (Chair)	J.C. Dumas
Japon	JAEA, CRIEPI	M. Kurata	T. Ogata
Netherlands	NRG	R. Mania	G.-J. de Haas
Rep. of Korea	KAERI	B.-O. Lee	J.-H. Kim
USA	DOE	T. Besmann (Vice-Ch.)	P. Turchi

Consultant: N. Dupin, Calcul Thermodynamique, France  
Coordinator: OECD-NEA (S. Massera)

Remarks and comments on this documentation and on the thermodynamic database are welcome. We thank you to ask for the authorization in case where you would like to communicate this documentation and/or the database to any other person. The database and the documentation cannot be modified. This documentation uses javascript. You must allow it in order to get it work properly.  
Current version: V6 2015 September 30th

### TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home Introduction Models Phases **Systems**

Elements  
Assessed binary systems  
Assessed ternary systems  
Higher order systems  
Systems with Ag, Al, Am, Ar, B, Ba, C, Ca, Ce, Cr, Cs, Fe, Gd, H, He, I, La, Mg, Mo, N, Nb, Nd, Ni, Np, O, Pd, Pu, Re, Rh, Ru, Si, Sr, Ta, Tc, Te, Th, Ti, U, V, W, Zr  
Periodic table

**Ternary systems**  
The assessed ternary systems defined by the database are listed hereunder by alphabetical order. At the current state of development of the database, only a few is assessed.

Al-Ca-O Al-Cr-O Al-Fe-O Al-Mg-O Al-O-Si Al-O-U Al-O-Zr  
Am-O-Pu  
B-C-Fe B-C-U B-C-Zr B-Fe-Zr B-H-O B-Pu-U  
Ba-Mo-O Ba-O-U Ba-O-Zr  
C-Mo-Re C-Mo-Si C-Mo-Ti C-Mo-U C-N-Ti C-N-U C-O-Pu C-O-U C-Pu-U C-Pu-W C-Re-U  
C-Re-W C-Si-Ti C-Si-U C-U-W C-U-Zr  
Ca-Fe-O Ca-Mg-O Ca-O-Si Ca-O-U Ca-O-Zr Ca-Si-U Ca-Si-Zr  
Ce-Fe-Nd Ce-O-U  
Cr-Fe-O Cr-Fe-Zr  
Cs-Mo-O Cs-O-U Cs-O-Zr  
Fe-O-Si Fe-O-U Fe-O-Zr Fe-U-Zr  
Gd-O-U  
La-O-U  
Mg-O-Si Mg-O-U Mg-O-Zr  
Mo-O-U Mo-Pd-Rh Mo-Pd-Ru Mo-Rh-Ru  
Nb-O-U  
Nd-O-U  
Ni-O-U  
O-Pu-U O-Pu-Zr O-Si-U O-Si-Zr O-Sr-U O-Sr-Zr O-U-Zr  
Pd-Rh-Ru  
Pu-U-Zr

Thus over 10660 ternary systems, 72 systems are assessed in the current database.