PLEIADES ALCYONE 3.5D simulation of a power ramp including OpenCalphad fuelthermochemistry with TAF-ID

C. Introïni, J. Sercombe, C. Gueneau, P. Goldbronn

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DE LA RECHERCHE À L'INDUSTRIE

NuFuel-MMSNF 2019 Workshop

Work done with support of the PLEIADES team and B. Sundman OpenCalphad

3 novembre 2019

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Plan

- **Context and objectives**
  - Industrial context
  - On the use of thermochemistry with TBASE and TAF-ID in PLEIADES ALCYONE 2.1
  - Towards validated multi-dimensional simulations with TAF-ID
- **TAF-ID *vs.* TBASE database**
  - 3.5D ALCYONE simulations of a short holding period power ramp
- **Conclusions & Future works**

Industrial context

Iodine-Stress Corrosion Cracking during Pellet-Cladding Interaction (PCI/I-SCC)

- One of the physical phenomena of major interest for cladding design and long term operation of Pressurized Water Reactors (PWRs)
- Chemistry of volatile fission products (iodine, cesium, tellurium) is of some importance with regards to PCI/I-SCC failures

  B. Baurens, et al., (2014). 3D thermo-chemical–mechanical simulation of power ramps with ALCYONE fuel code, J. Nucl. Mater. 452, 578-594.
- A "realistic" modelling of this phenomenon needs a precise description of FPs thermochemistry and their migration/release in the fuel under irradiation

Numerical simulation of Iodine-Stress Corrosion Cracking phenomenon

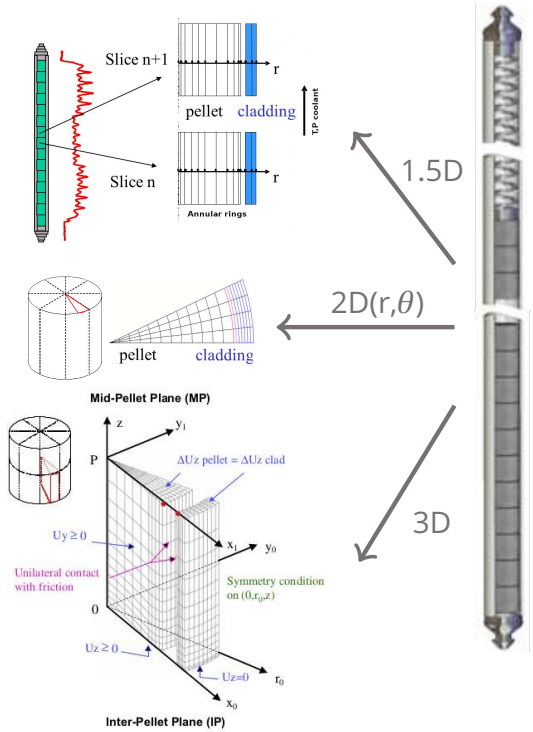
- Requires to have accurate, efficient and robust thermo-mechanical and thermochemical solvers

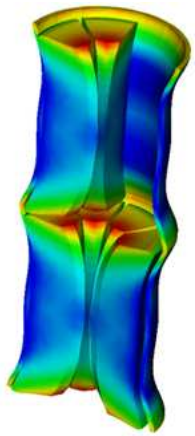
⇒ **Use of the validated PLEIADES/ALCYONE 2.1 fuel performance code**

V. Marelle & al. , "New developments in ALCYONE 2.0 fuel performance code", Top Fuel, Boise ID. (2016)

A fuel performance code for Pressurized Water Reactors fuel rods

- Co-developed by CEA, EDF, Framatome
- Provides a multidimensional modeling for detailed analyses of PWR fuel elements behavior under irradiation
  - 1.5D scheme : rod discretized in axial segments
  - 2D(r,θ) scheme : mid-pellet plane of a pellet fragment
  - 3D scheme : one quarter of a pellet fragment
  - 3.5D scheme : rod discretized in axial pellet fragments
- Using the Finite Elements code CAST3M (CEA) to solve the thermo-mechanical problem
- Major phenomena considered in the 1D, 2D and 3D schemes





Fuel pellet

Power deposition, Heat conduction, Fission Gas Release, Diffusion of Fission Gas, Creep & cracking of the fuel pellet, Pellet densification, Pellet FG-induced swelling, Relocation of pellet fragments (1D), Properties depending on irradiation, thermochemistry with TBASE and TAF-ID

Cladding material

Heat conduction, Irradiation creep, Thermal creep, Plasticity, Properties depending on irradiation

Pellet-Cladding interface

Heat convection, Contact with friction (3D), Pressure update (FG release, rodlet deformation)

Integration of an accurate thermochemical modeling of irradiated fuel in PLEIADES

- A significant work done since the early 2010s to be able to simulate I-SCC
- ANGE (*Advanced Numeric Gibbs Energy minimizer*), a modified version of SOLGASMIX
  - ✓ Integrated in PLEIADES/ALCYONE 1.4 as a first step towards I-SCC simulations *B. Baurens, et al., (2014). 3D thermo-chemical–mechanical simulation of power ramps with ALCYONE fuel code, J. Nucl. Mater. 452, 578-594.*
  - ✓ Coupled with oxygen thermal distribution model *P. Konarski & al. , 3D Simulation of power ramps with ALCYONE including fuel thermochemistry and oxygen thermodiffusion, Top Fuel (2018)*
  - – Using the associate species description for (U,Pu,PF)$O_{2\pm x}$ solid solution *T.M. Besmannn, (2012), Computational Thermodynamics : Application to Nuclear Materials, Compr. Nucl. Mater. 1 455–470* and thermodynamic functions from the TBASE database *E.H.P. Cordfuncke, R.J.M. Konings, (1993), J. Phase Equilibria 14 : 457*
  - ✗ Cannot be used to solve chemical systems based on the Compound Energy Formalism as proposed in the TAF-ID database (`https://www.oecd-nea.org/science/taf-id/`) *C. Guéneau et al., (2011). Thermodynamic modelling of advanced oxide and carbide nuclear fuels : Description of [-0.2cm]the U–Pu–O–C systems, J. Nucl. Mater., 419, 145-167*

. . . being able to use the TAF-ID (*Thermodynamics of Advanced Fuels - International Database*)

- – OECD-NEA project aiming at making a comprehensive, internationally recognised and quality-assured database of phase diagrams and thermodynamic properties for nuclear advanced fuels (Generation II-III reactors, Generation IV systems)

TBASE database

- 24 elements of the periodic table
- Associate species description for the oxide (*i.e.* sub-lattice description, cristalline structure)
- ~ 100 stoichiometric compounds
- No description of the liquid phase diagram

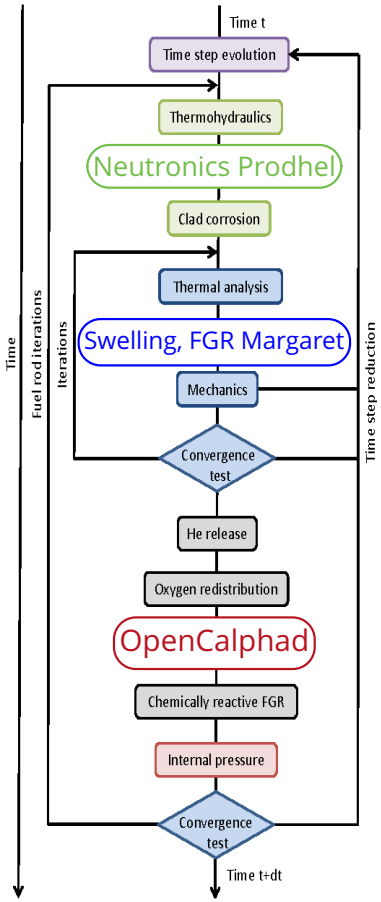
vs.

TAF-ID database

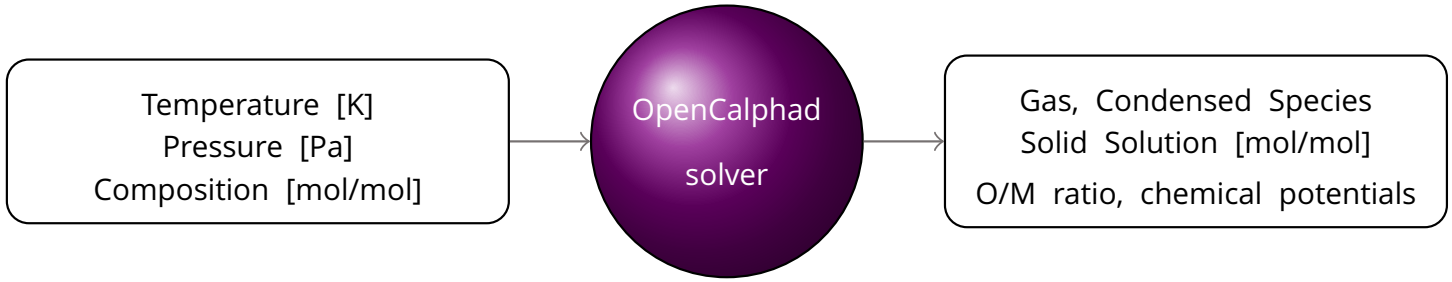
- 41 elements of the periodic table
- Compound Energy Formalism for the oxide (*i.e.* sub-lattice description, cristalline structure)
- ~ 150 stoichiometric phases
- Description of the liquid phase diagram (interesting for high temperatures)

- ✓ TAF-ID database provides a more complex description of the irradiated fuel (more complicated models, possible phases greater in number than in the TBASE database) and enables to describe liquid phase diagram

OpenCalphad a free, efficient and robust thermo-chemical solver



- Developed by B. Sundman http://www.opencalphad.org/
- Can use the TBASE and OECD-NEA TAF-ID databases
- OpenCalphad 5.0 integrated in PLEIADES/ALCYONE 2.0 (CeCILL-C license)
  - $\forall t$, OpenCalphad calculations are done at each node after multiphysics convergence loop



  - Initial composition is given by PRODHEL neutronics solver and it is assumed that only gas species formed are released from fuel proportionaly to inert FG flux given by MARGARET

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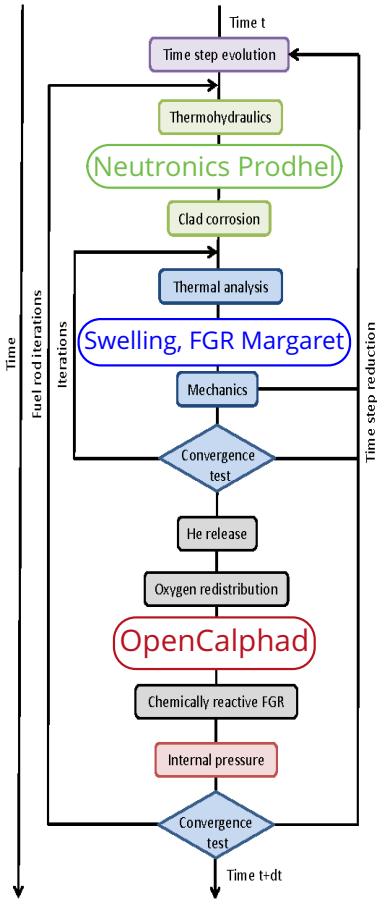

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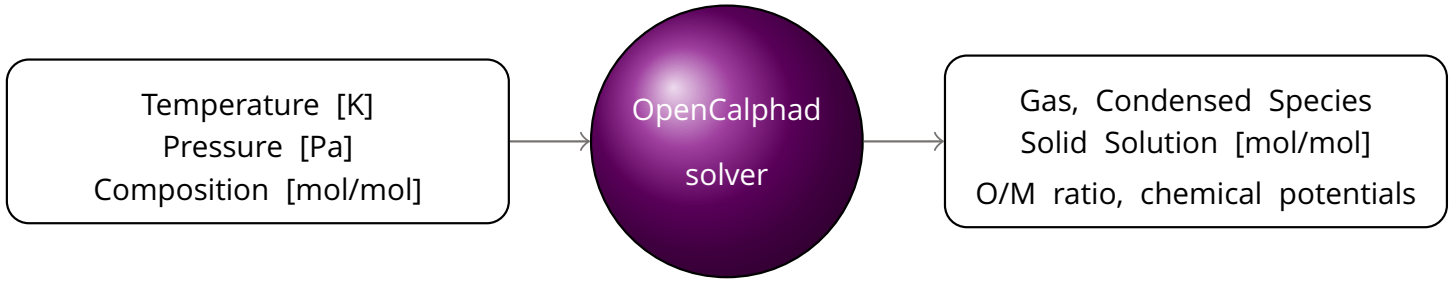

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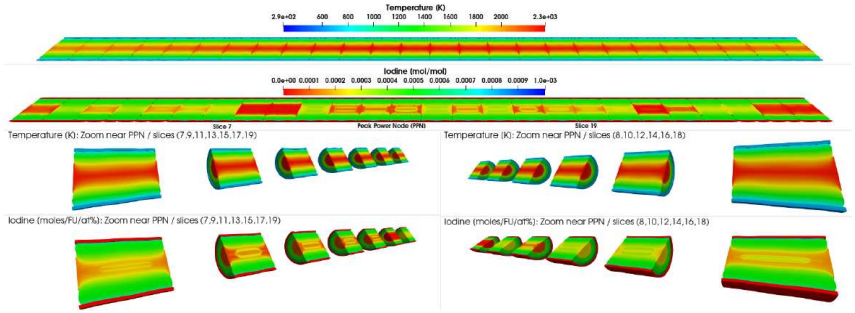
⇒ **ALCYONE/OpenCalphad is much faster than ALCYONE/ANGE with TBASE thanks to numerical strategies reducing the CPU time**

⇒ **Capacity and robustness of ALCYONE OpenCalphad to simulate multi-dimensional power transients with TAF-ID database**



3.5D ALCYONE simulation with TAF-ID
(C. Introïni *& al.* , NuMat2018, Seattle)

⇒ **work to be published**

OpenCalphad with TAF-ID : an advanced numerical scheme of thermochemistry in the PLEIADES plateform

- Interesting and promising...
  - to have a more complex description of the irradiated fuel in nominal and accidental conditions)
  - to contribute to the analyze and the interpretation of experimental programs (*e.g.* VERDON and VERCORS experimental programs)

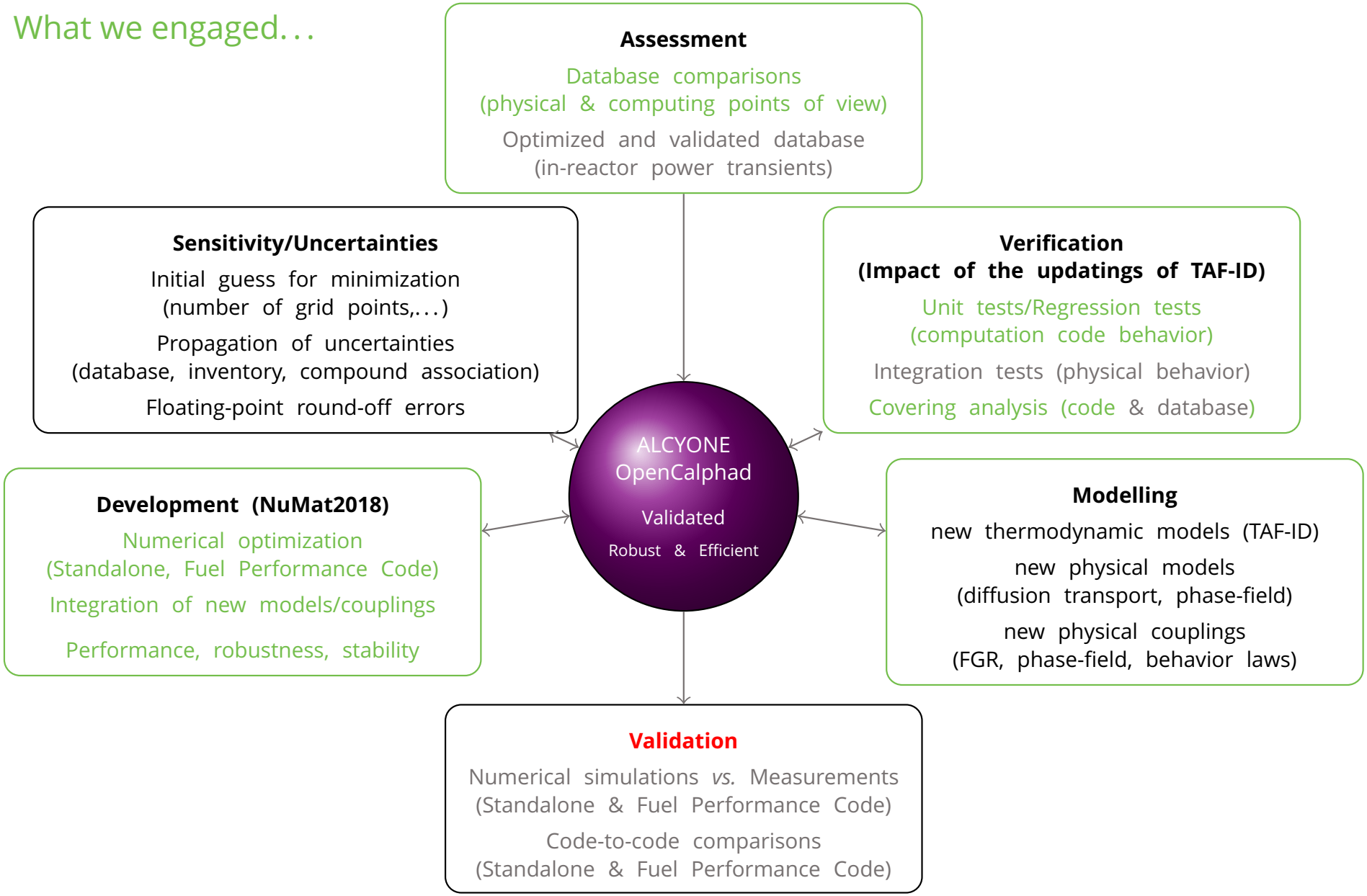
    E. Geiger et al., (2019). Modelling nuclear fuel behaviour with TAF-ID : Calculations on the VERDON-1 experiment, representative of a nuclear severe accident, J. Nucl. Mater., 522, 294-310

    A. Germain, Impact of local chemical equilibria in the fuel on fission products release : from accidental conditions to core melting, Thesis (2018-2021)
  - to simulate complex multi-physics problems involving, for example, species transport mechanisms in multiphase multicomponent system (with Soret and Dufour effects)

- **...but in order to be able to perform validated multi-dimensional simulations of in-reactor power transients, a major and rigorous work**

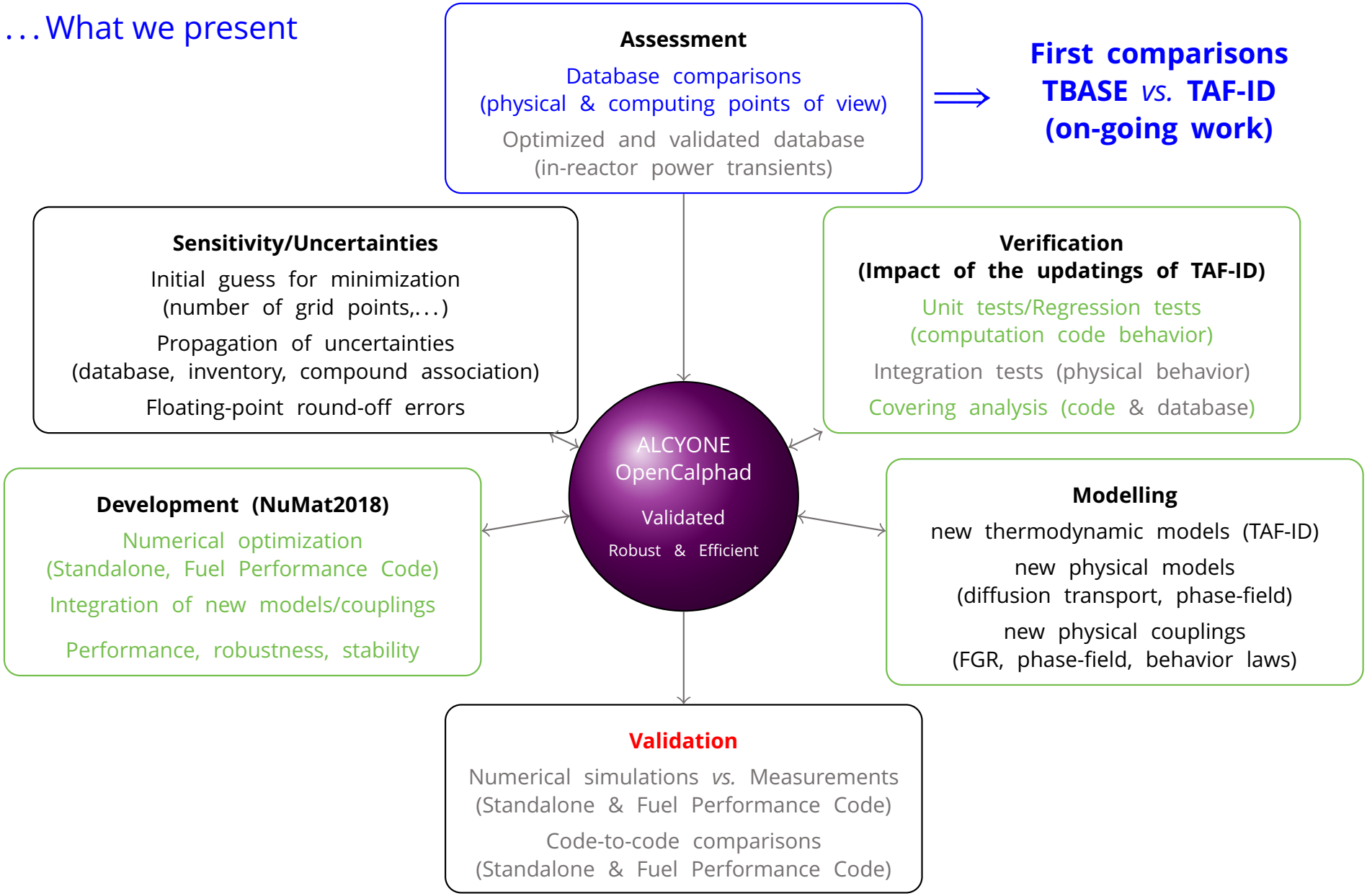
Towards validated multi-dimensional simulations with TAF-ID

What we engaged. . .



Towards validated multi-dimensional simulations with TAF-ID

. . . What we present



TAF-ID *vs.* TBASE database

3.5D ALCYONE simulations of a short holding period power ramp

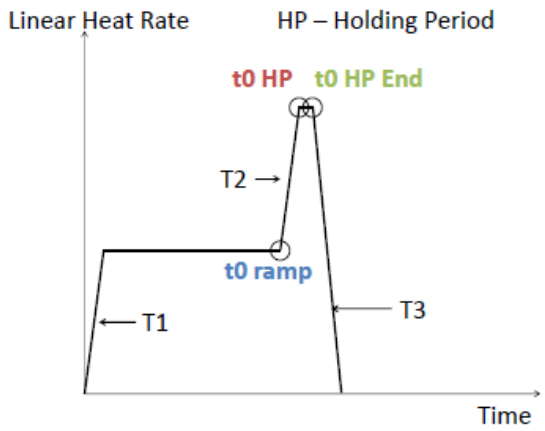
Commissariat à l'énergie atomique et aux énergies alternatives - www.cea.fr

3.5D ALCYONE simulations of a short holding period power ramp

Characteristics of the power ramp

- Rodlet power ramped in the OSIRIS reactor
  - Fuel material : UO_2 / Cladding material : Zircaloy-4

Max. LHR [W/cm]	Cond. Period [h]	Cond. Period Power [W/cm]	**Holding Period** [s]	T1 [min]	T2 [s]	T3 [s]
520	16	180	90	4.9	192	6



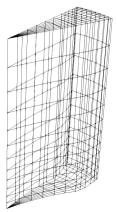
Characteristics of the 3.5D PLEIADES/ALCYONE simulations

B. Baurens & al. , (2014). 3D thermo-chemical–mechanical simulation of power ramps with ALCYONE fuel code, J. Nucl. Mater. 452, 578-594

P. Konarski & al. , 3D Simulation of power ramps with ALCYONE including fuel thermochemistry and oxygen thermodiffusion, Top Fuel (2018)

- **OpenCalphad fuel thermochemistry with TAF-ID V8 (8-th CEA version, 2018) and TBASE**
- Fission Gas Release model MARGARET and Neutronics model PRODHEL
- Some computing informations
  - 27 slices over 27 CPUs, 1/32 fuel pellet per slice and 455 nodes per slice
  - **577395 equilibrium calculations done with OpenCalphad over 47 time-steps**
  - **Successful calculations : 99.9% with TBASE and 99.4% with TAF-ID**

Element	Representative element	Family
He+Xe+Kr	He	Inert fission gas and volatile fission products
Cs+Rb	Cs	
I+Br	I	
Te+Se+Ge+As	Te	
Ba+Sr	Ba	Stable oxides
Zr+Nb	Zr	
Mo	Mo	
Ru+Tc+Rh	Ru	Metallic fission products
Pd+Sn+Sb	Pd	
Ce+Pr	Ce	Fission products and actinides in solid solution in UO2
Eu+Sm	Eu	
La+Y	La	
Gd+Nd+Pm	Gd	
Pu+Np+Am+Cm	Pu	



1/32 fuel pellet

455 nodes/slice (coarse mesh)

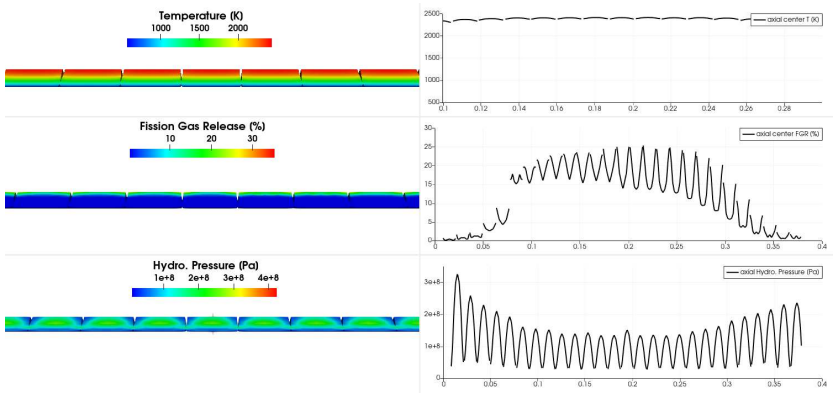
3.5D ALCYONE simulations of a short holding period power ramp

Temperature, Hydrostatic Pressure and Fission Gas Release (here, illustrated during the Holding Period)

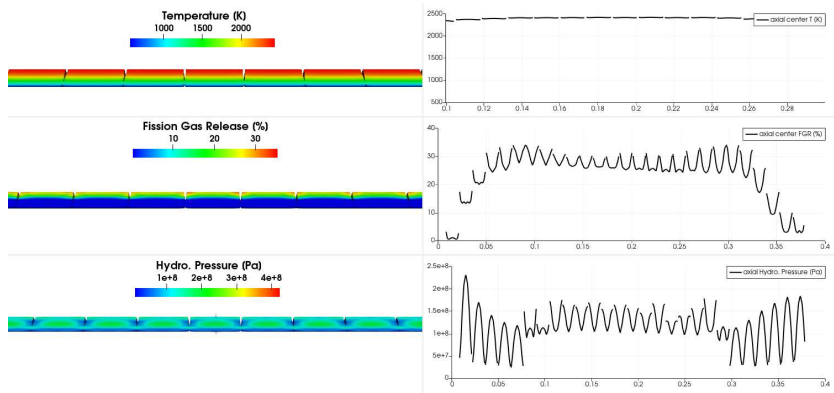
- Good agreement of the results with measurements and the predicted results published by *B. Baurens & al. , J. Nucl. Mat. 452 (2014)* and *P. Konarski & al. , Top Fuel (2018)*
- Temperature
  - axial temperature in the center of the fuel pellet reaches ~ 2400K during the Holding Period (HP)
- Hydrostatic Pressure and inert Fission Gas Release (MARGARET)
  - Important axial pressure gradients in the central part of the fuel between mid-pellet and inter-pellet planes (MP-IP)
  - The lower the hydrostatic pressure, the higher the Fission Gas Release (see, for example, values at IP plane)

Axial profiles at the center of the fuel of T (top), FGR (middle), P (bottom)
Visualization near the PPN

Start of the HP (axial profiles)



End of the HP (axial profiles)



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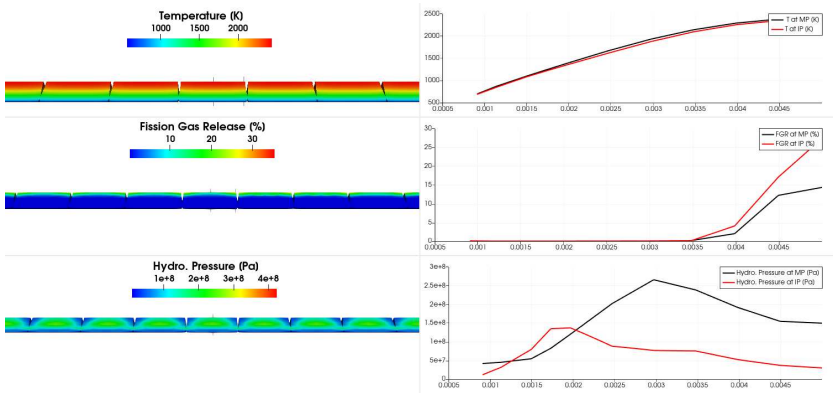
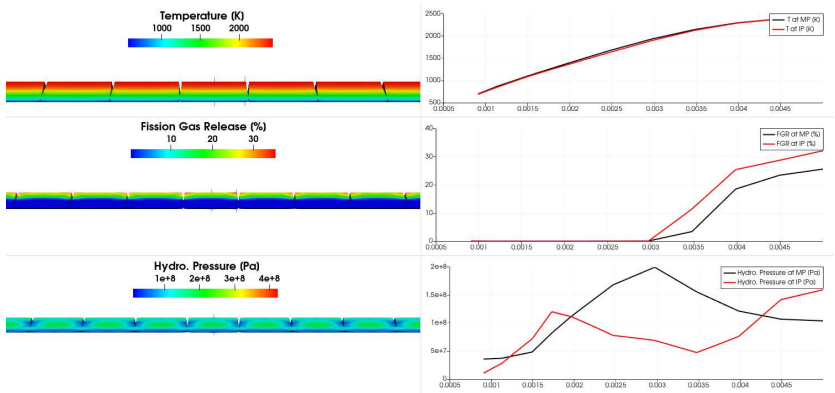
- Temperature
  - axial temperature in the center of the fuel pellet reaches ~ 2400K during the Holding Period (HP)
  - Radial gradient≫Axial gradient ⇐ fuel/cladding gap closure during the Holding Period (HP)
- Hydrostatic Pressure and inert Fission Gas Release (MARGARET)
  - Important axial pressure gradients in the central part of the fuel between mid-pellet and inter-pellet planes (MP-IP)
  - The lower the hydrostatic pressure, the higher the Fission Gas Release (see, for example, values at IP plane)
  - Increase of the inert Fission Gas Release from the center of the fuel towards the periphery during the Holding Period

Radial profiles of T (top), FGR (middle), P (bottom) from the center of the fuel (right) towards the periphery (left)
Visualization near the PPN and radial profiles done at the center of the rod

Start of the HP (radial profiles)



End of the HP (radial profiles)



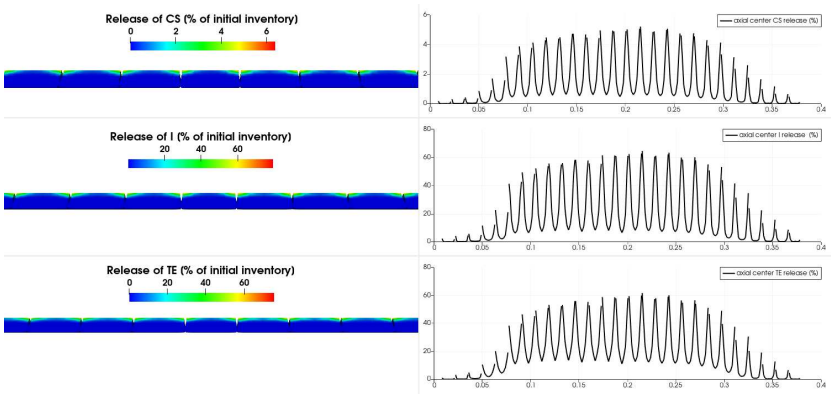
3.5D ALCYONE simulations of a short holding period power ramp

Volatile Fission Products (CS, I, Te) Release (OpenCalphad calculation with TBASE database)

- Good agreement of the results with the predicted results published by *B. Baurens & al. , J. Nucl. Mat. 452 (2014)* and *P. Konarski & al. , Top Fuel (2018)* (better agreement could be obtained with a finer mesh)
- Effect of the non-uniform axial pressure distribution on the release of Cs (top), I (middle), Te (bottom) : axial gradient between the MP plane (low values) and the IP plane (high values)

Axial profiles at the center of the fuel of Cs (top), I (middle), Te (bottom)
Visualization near the PPN

Start of the HP (TBASE results)



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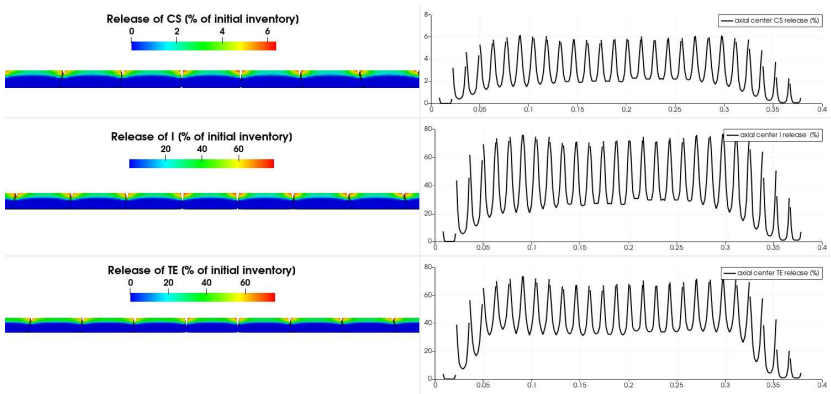

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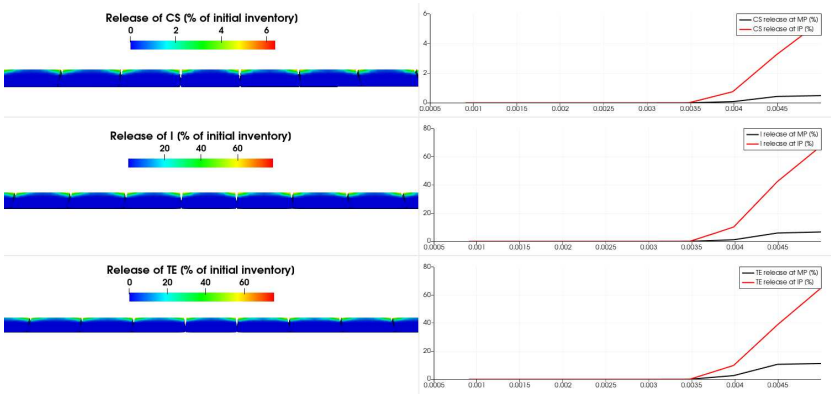
Radial profiles of Cs (top), I (middle), Te (bottom) from the center of the fuel (right) towards the periphery (left)
Visualization near the PPN and radial profiles done at the center of the rod

Start of the HP (TBASE results)



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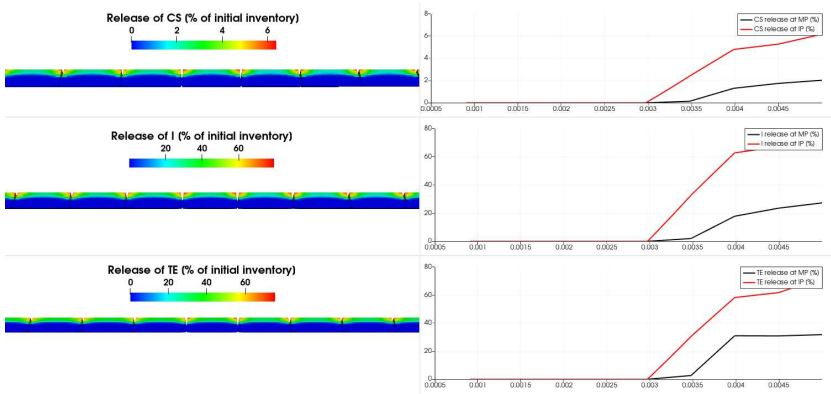


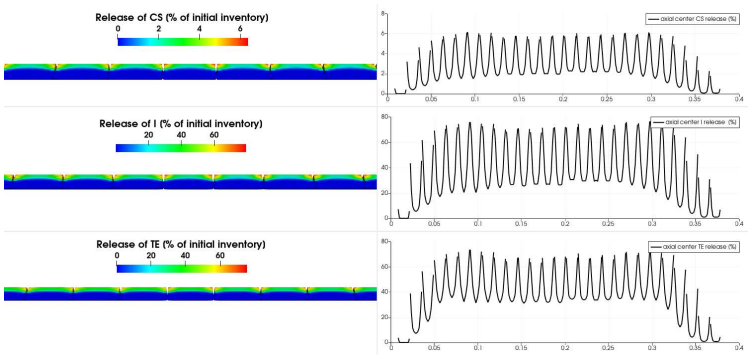
- The general trend observed on the release of volatile FPs is consistent with measurements
  - Increase of FPs release from the center of the pellet towards the periphery during the HP
  - Important release of Iodine but underestimation of Tellurium release in comparison with experimental measurements
  - Low release of Cesium (consistent with B. Baurens *& al.*) explained by an effect of oxygen thermal diffusion not simulated

3.5D ALCYONE simulations of a short holding period power ramp

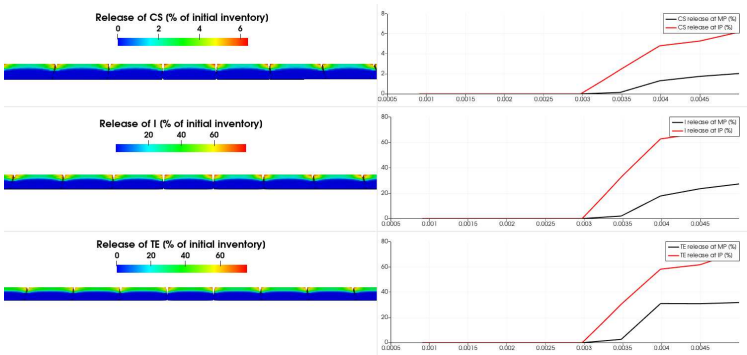
Volatile Fission Products (CS, I, Te) Release : TBASE database *vs.* TAF-ID database (at the end of the HP)

- ✓ General trend of the release of volatile FPs calculated with TAF-ID consistent with the one observed with TBASE (effect of the pressure on axial profiles, higher release from the center)

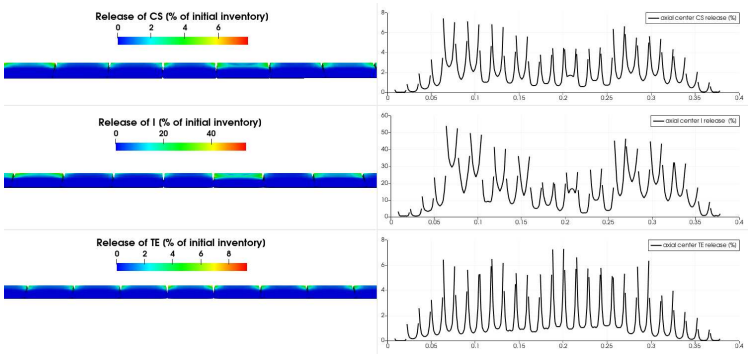
TBASE axial profiles : Cs (top), I (mid), Te (bottom)



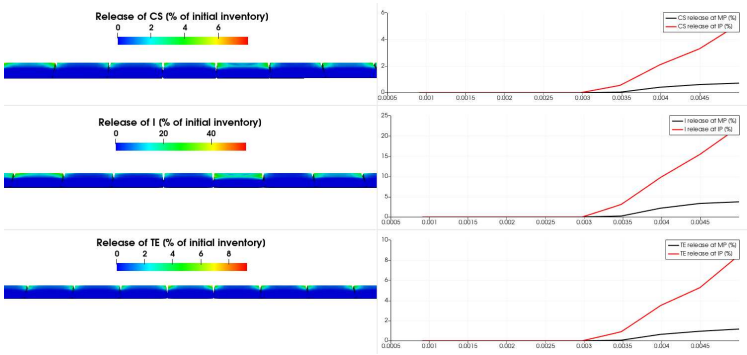
TBASE radial profiles : Cs (top), I (mid), Te (bottom)



TAF-ID axial profiles : Cs (top), I (mid), Te (bottom)



TAF-ID radial profiles : Cs (top), I (mid), Te (bottom)

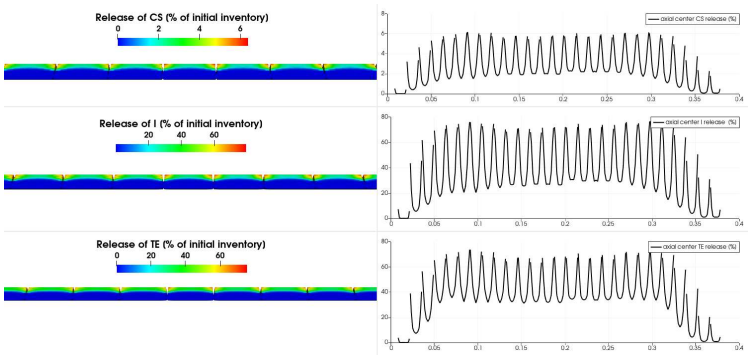


3.5D ALCYONE simulations of a short holding period power ramp

Volatile Fission Products (CS, I, Te) Release : TBASE database *vs.* TAF-ID database (at the end of the HP)

- ✓ General trend of the release of volatile FPs calculated with TAF-ID consistent with the one observed with TBASE (effect of the pressure on axial profiles, higher release from the center)
- ✗ Axial distribution of the release of volatile FPs is less uniform with TAF-ID than with TBASE
- ✗ Release of volatiles FPs calculated with TAF-ID significantly lower than those calculated with TBASE

TBASE axial profiles : Cs (top), I (mid), Te (bottom)



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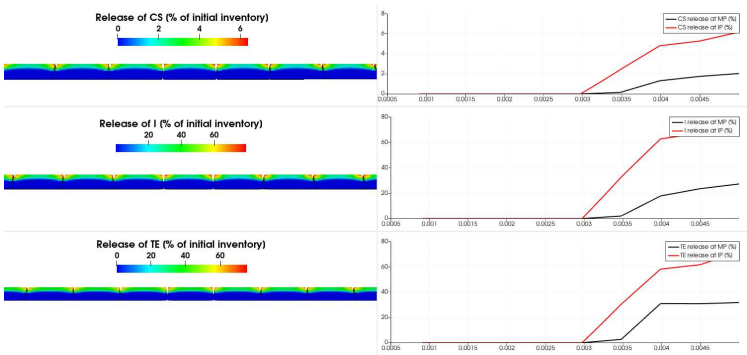

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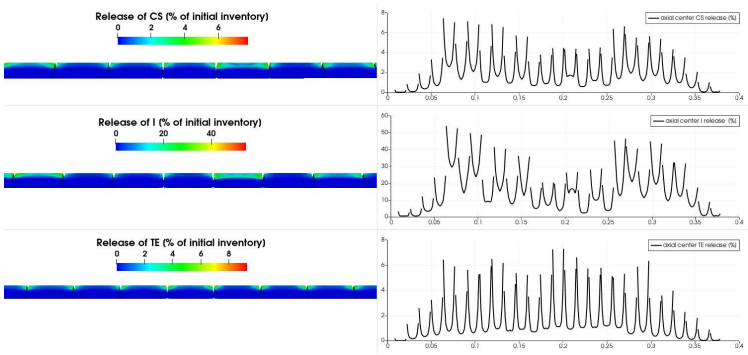

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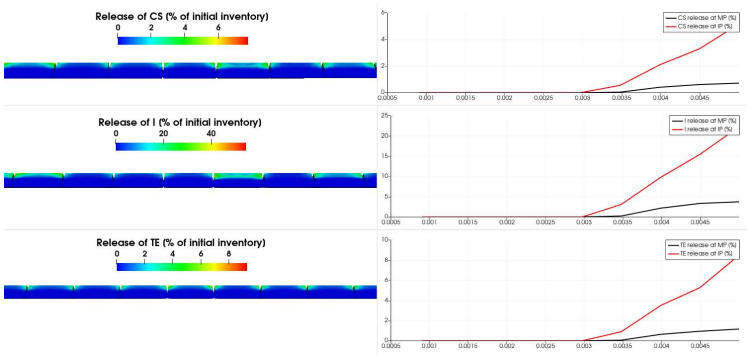

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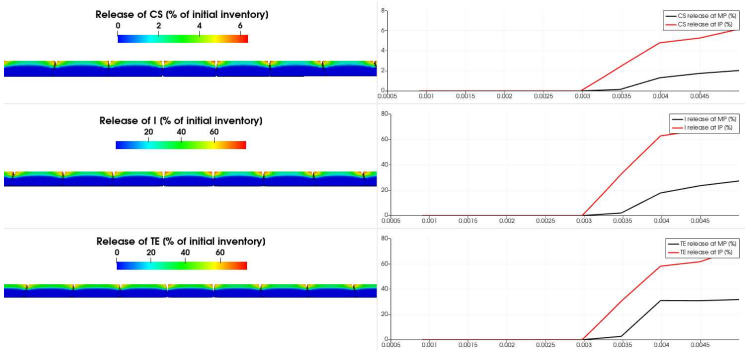
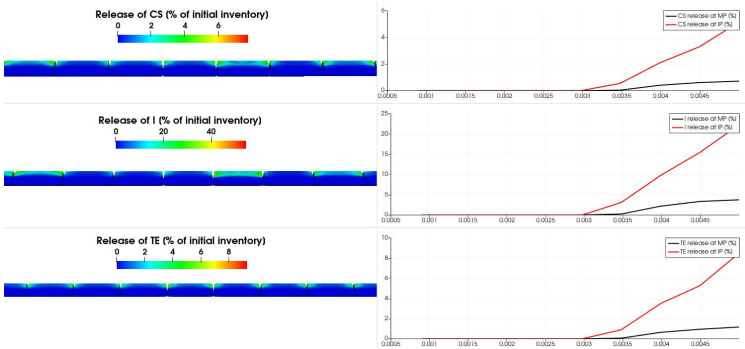
- ✗ Axial distribution of the release of volatile FPs is less uniform with TAF-ID than with TBASE
- ✗ Release of volatiles FPs calculated with TAF-ID significantly lower than those calculated with TBASE
- ► On these radial profiles, depending on the position in the fuel, we may have the following trends :
  - release of CS with TAF-ID ~2 times lower than with TBASE
  - release of I with TAF-ID ~3-6 times lower than with TBASE
  - release of TE with TAF-ID ~15 times lower than with TBASE

TBASE radial profiles : Cs (top), I (mid), Te (bottom)



TAF-ID radial profiles : Cs (top), I (mid), Te (bottom)



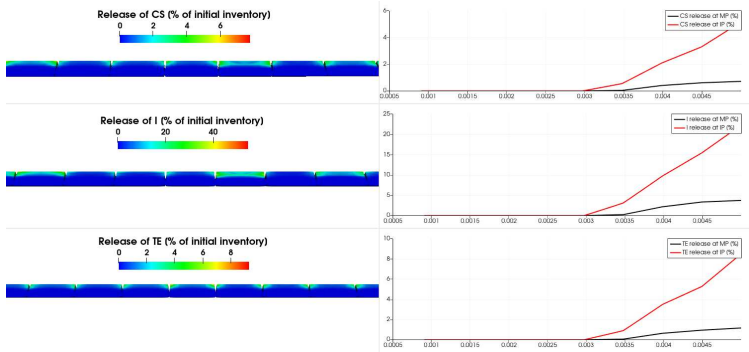
3.5D ALCYONE simulations of a short holding period power ramp

Volatile Fission Products (CS, I, Te) Release : TBASE database *vs.* TAF-ID database (at the end of the HP)

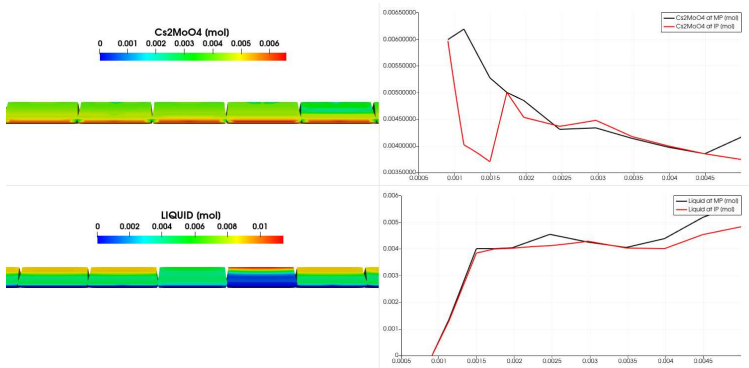
- ✓ General trend of the release of volatile FPs calculated with TAF-ID consistent with the one observed with TBASE (effect of the pressure on axial profiles, higher release from the center)
- ✗ Axial distribution of the release of volatile FPs is less uniform with TAF-ID than with TBASE
- ✗ Release of volatiles FPs calculated with TAF-ID significantly lower than those calculated with TBASE
- ► On these radial profiles, depending on the position in the fuel, we may have the following trends :
  - release of CS with TAF-ID ~2 times lower than with TBASE
  - release of I with TAF-ID ~3-6 times lower than with TBASE
  - release of TE with TAF-ID ~15 times lower than with TBASE
- ► How to explain these results? 🤔
  - from the presence of liquid phases (miscibility gap found)?
  - here, release of volatiles FPs proportional to inert FG flux

    ⇒ Cs, I, Te in liquid not taken into account in the release
  - from a detailed analysis of the composition of the gas phase and from the evolution of the other phases such as, for example, Cs_2MoO_4 ?

Cs, I, Te - End of the HP (TAF-ID results)



LIQUID and Cs2MoO4 - End of the HP (TAF-ID results)



3.5D ALCYONE simulations of a short holding period power ramp

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    ⇒ Cs, I, Te in liquid not taken into account in the release
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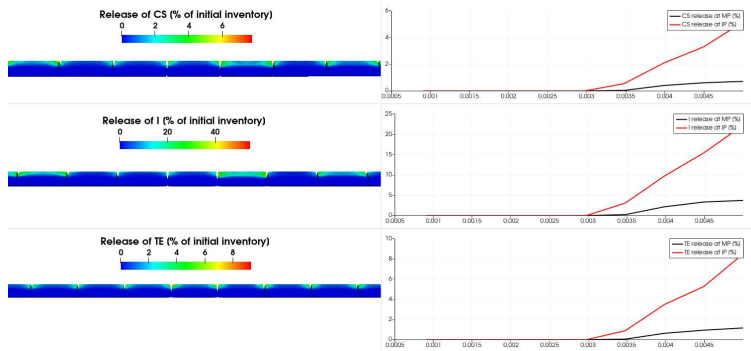
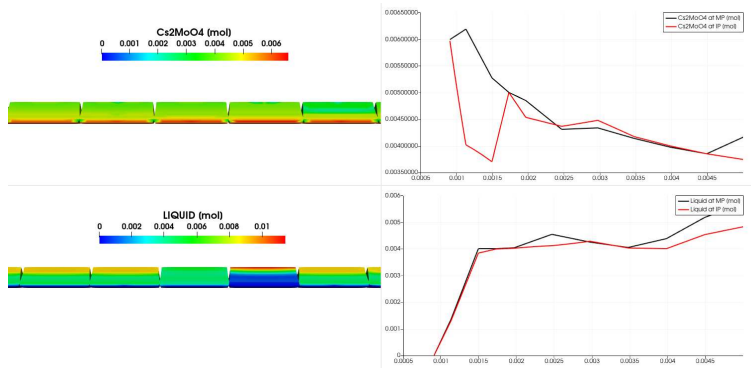
⇒ **Detailed analysis is in progress . . .**

Cs, I, Te - End of the HP (TAF-ID results)



LIQUID and Cs2MoO4 - End of the HP (TAF-ID results)

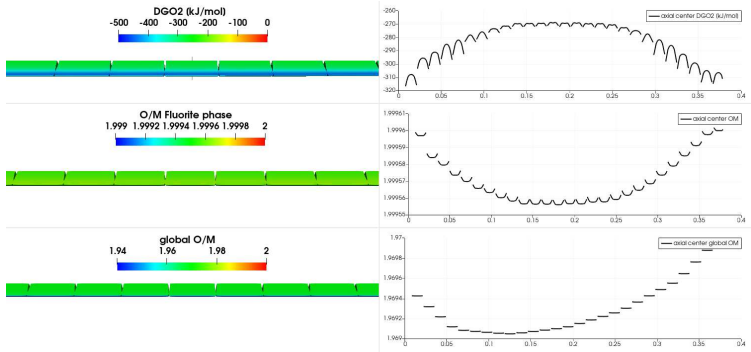


3.5D ALCYONE simulations of a short holding period power ramp

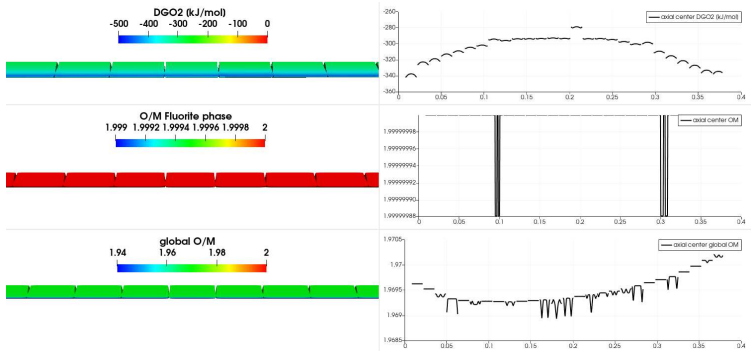
Oxygen potential ΔGO_2 (top), Oxygen-to-Metal ratio O/M (in the fluorite phase (middle) and in the bulk (bottom)) : TBASE database *vs.* TAF-ID database (at the end of the HP)

- Increase of the ΔGO_2 during the HP (here, focus on the end of HP)
- Axial distribution of ΔGO_2 consistent with temperature axial profile (TBASE and TAF-ID)
- Axial distribution of ΔGO_2 is ~10% higher with TAF-ID than with TBASE
- Axial profile of the local O/M obtained with TBASE consistent with temperature profile (the higher temperature, the higher solulibilty of FPs)
- No effect of the temperature with TAF-ID : local O/M close to 2
- Bulk O/M axial profile consistent with linear power profile (TBASE and TAF-ID)

End of the holding period (TBASE results)



End of the holding period (TAF-ID results)



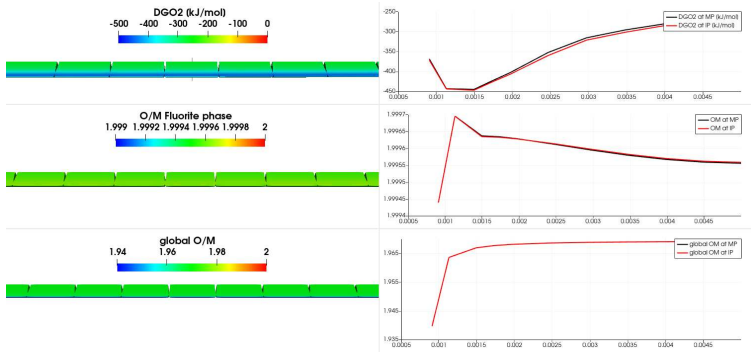
3.5D ALCYONE simulations of a short holding period power ramp

Oxygen potential ΔGO_2 (top), Oxygen-to-Metal ratio O/M (in the fluorite phase (middle) and in the bulk (bottom)) : TBASE database *vs.* TAF-ID database (at the end of the HP)

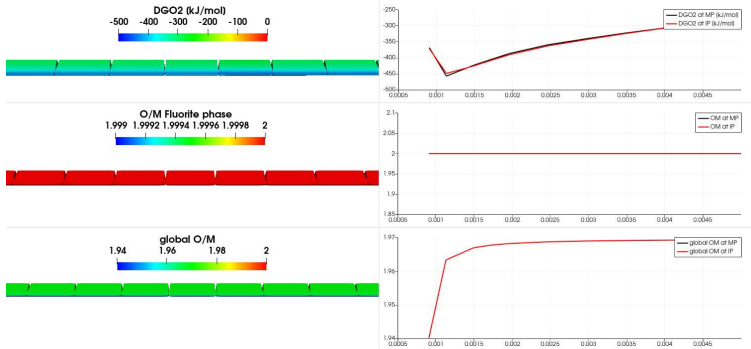
- Except near the top and the bottom of the rodlet, the ΔGO_2, the local O/M and the bulk O/M radial profiles are similar at IP and MP due to a quasi-constant temperature
- Similar radial profiles of ΔGO_2 and of the bulk O/M obtained with TBASE and TAF-ID
  - ΔGO_2 decreases from the center of the pellet towards the periphery and then increases in the RIM region
  - the bulk O/M decreases slightly until the RIM region where a more important decrease is predicted
- Local O/M radial profiles obtained with TBASE consistent with the predicted ΔGO_2 radial profile
- Local O/M radial profiles obtained with TAF-ID close to 2

  ⇒ **Work is in progress to understand this results**

End of the holding period (TBASE results)



End of the holding period (TAF-ID results)



- **TAF-ID results close to TBASE results (except for local O/M)**
  - Good agreement of the results with *P. Konarski & al. , Top Fuel (2018)* (without effects associated with oxygen thermal diffusion not simulated here)

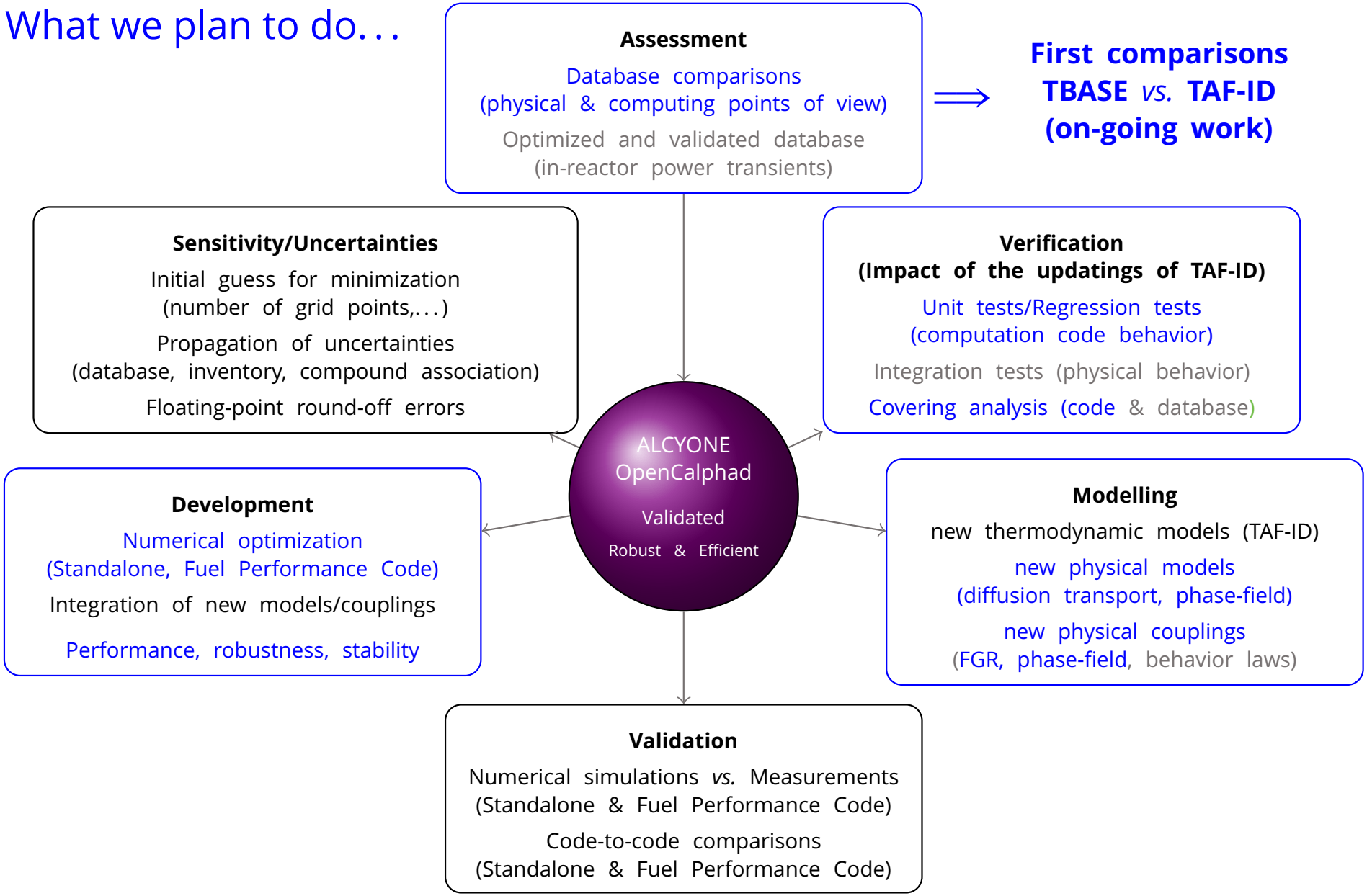
Conclusions

Towards validated multi-dimensional simulations with TAF-ID

- **Overview of what we should perform to do validated multi-dimensionsal simulations with TAF-ID and what we engaged to acheive this challenging objective**
- **First comparisons between TBASE database and TAF-ID have been presented**
  - 3.5D ALCYONE simulations of a short holding power ramp
    - ✓ **In that case, the results are satisfactory and consistent with those already published**
    - ✓ **However, TAF-ID yields volatile FPs lower than those calculated with TBASE and a local O/M close to** 2
    - ⇒ Work must be followed to well understand why the release of volatile PFs predicted by TAF-ID is lower than the one calculated with TBASE database
- **First promising results have been obtained but a significant and rigorous work must be conducted, mainly to understand the strengths and the weaknesses of TAF-ID compare to TBASE database as well as to explain differences observed on the results of the simulations of in-reactor power transients done with both thermodynamic databases**

Works foreseen in 2020

What we plan to do...



Works foreseen in 2020

Continuation of the optimization work to reduce the CPU time with TAF-ID

- Upcoming update of the numerical strategies with an increase in robustness and in stability as well as an improvement of the parallel implementation
- Numerical optimization of the OpenCalphad solver (in collaboration with B. Sundman)

Integration of a phase-field solver in the PLEIADES plateform

- Development of phase-field methods to simulate melting with thermal diffusion, oxygen thermal diffusion and local equilibrium calculations in the fuel of PWRs (PostDoc 2020)
  - Cahn-Hilliard/Allen-Cahn methods coupled with OpenCalphad thermochemical solver

    M.J. Welland, et al., (2011), Review of high temperature thermochemical properties and application in phase-field modelling of incipient melting in defective fuel, J. Nucl. Mater. 412, 342-349
- Numerical simulation of species diffusion by a phase-field method in multiphase non-stoichiometric oxide systems subjected to a temperature gradient (PhD, 2020-2023)
  - New step toward an advanced description of species transport mechanisms
  - Natural coupling with CALPHAD methods (TAF-ID) and use of diffusion properties depending on point defects *E. Moore, C. Guéneau, J.-P. Crocombette, Diffusion model of the non-stoichiometric uranium dioxide, Journal of Solid State Chemistry 203 (2013) 145–153*

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