REDUCTION OF RADIOLOGICAL ACCIDENT CONSEQUENCES

Title	Fuel behaviour modelling advancements
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Affiliation:	European Commission, DG Joint Research Centre, Karlsruhe
Event:	R2CA Summer School
When:	4-6 July 2023
Where:	ENEA Bologna

European Commission

Commission européenne

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Outline

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Mechanistic modelling of fission product behaviour
  - SCIANTIX
  - MFPR-F
- Model improvements for TRANSURANUS and FRAPTRAN codes

SCIANTIX

- Bounding the numerical error

- Introducing radioactive FP release

PhD of G. Zullo at POLIMI

SCIANTIX: ANS5.4 model implementation

- Intragranular part: based on Booth equation for diffusion in sphere

$$\frac{R}{B} = \frac{3}{R_{grain}}\sqrt{\frac{D}{\lambda}}\left[\coth\left(R_{grain}\sqrt{\frac{\lambda}{D}}\right) - \frac{1}{R_{grain}}\sqrt{\frac{D}{\lambda}}\right]$$

- Accounting for precursor in a simplified manner

$$\left(\frac{R}{B}\right)_{diff} = \frac{S}{V}\sqrt{\frac{\alpha D}{\lambda}}$$

$$\alpha = \left(\frac{\left(1-\frac{y}{x}\right)^3}{\left(1-\frac{y}{x}\right)^2}\right)^2, \; x = \sqrt{D_{\text{nuclide}}/\lambda_{\text{nuclide}}}, \; y = \sqrt{D_{\text{precursor}}/\lambda_{\text{precursor}}}$$

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Intergranular part based on Vintanza or Halden threshold: Bubble interconnection leads to incubation

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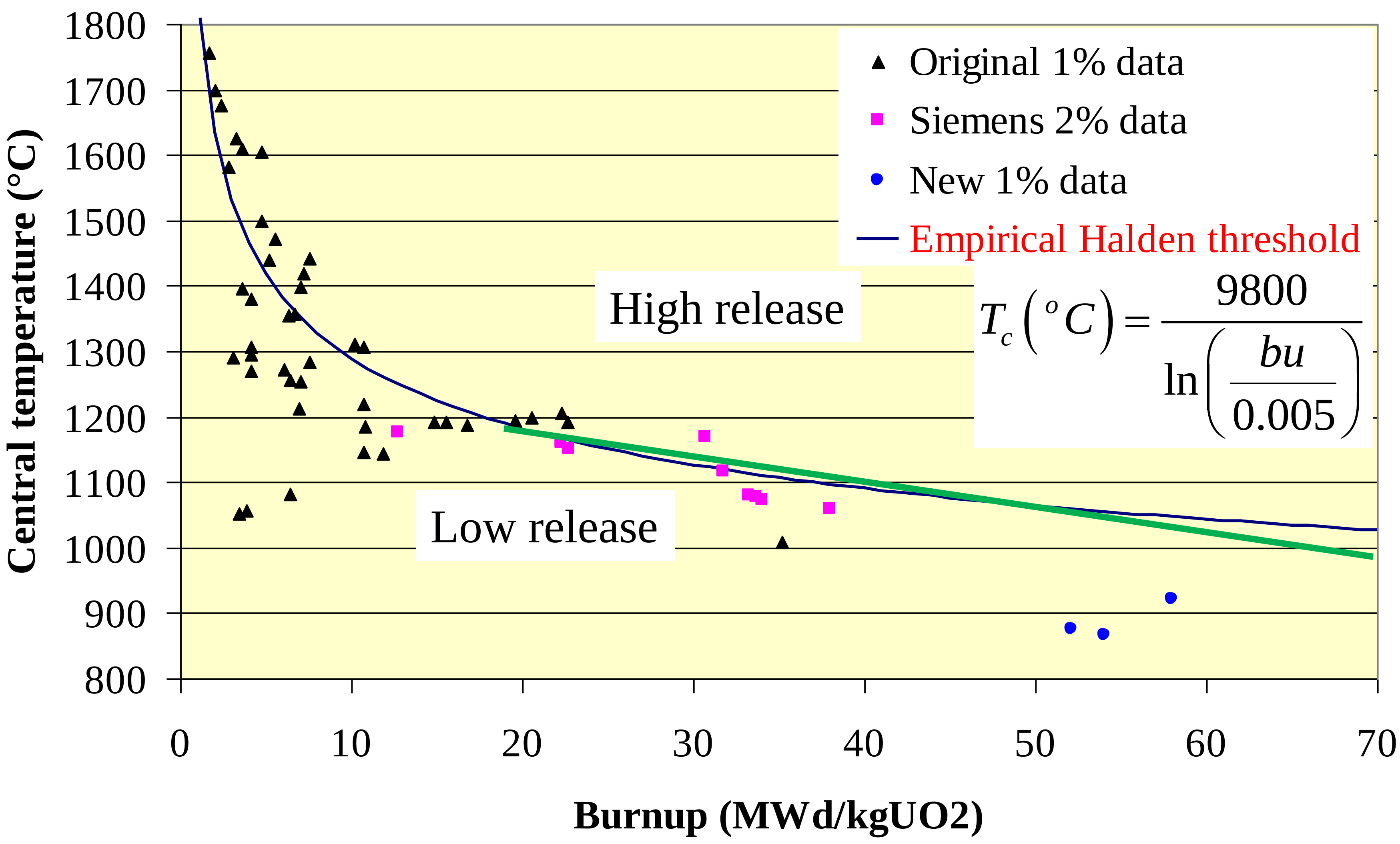

ANS5.4 approx. when Bu > 18MWd/kgHM

SCIANTIX: ANS5.4 model implementation

- Intergranular part: empirical model of T and burnup
  - Interconnection temperature (T_{IC}):
    - T_{IC} = Vitanza curve for bu <18.2 MWd/kgHM
    - Linear decrease beyond that burnup
  - (S/V)= 120 /cm for $T < T_{IC}$, 650 when $T > T_{IC}$
- Only applicable to steady-state conditions

SCIANTIX: ANS5.4 model improvement

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- Physics-based modelling of intergranular model of SCIANTIX for ANS5.4-2010, hence available in SCIANTIX and in the coupled code TRANSURANUS//SCIANTIX.
- Dynamics of the predicted release close to experimental results.
- Able to reproduce the release rate during sudden power variations, based on mechanistic approach.

CONTACT experiment outline

- Short rodlet of Zr-4 clad with 5 UO_2 Framatome pellets of typical 17x17 PWR design.
- Included in International Fuel Performance Experiments database (IFPE) of IAEA-NEA
- Objective

  Behaviour of fuel centerline temperature, pellet-clad gap, cumulative fractional release of stable fg and **release/birth of radioactive fg in the range 0-22 MWd/kgM and 0-40 kW/m)**

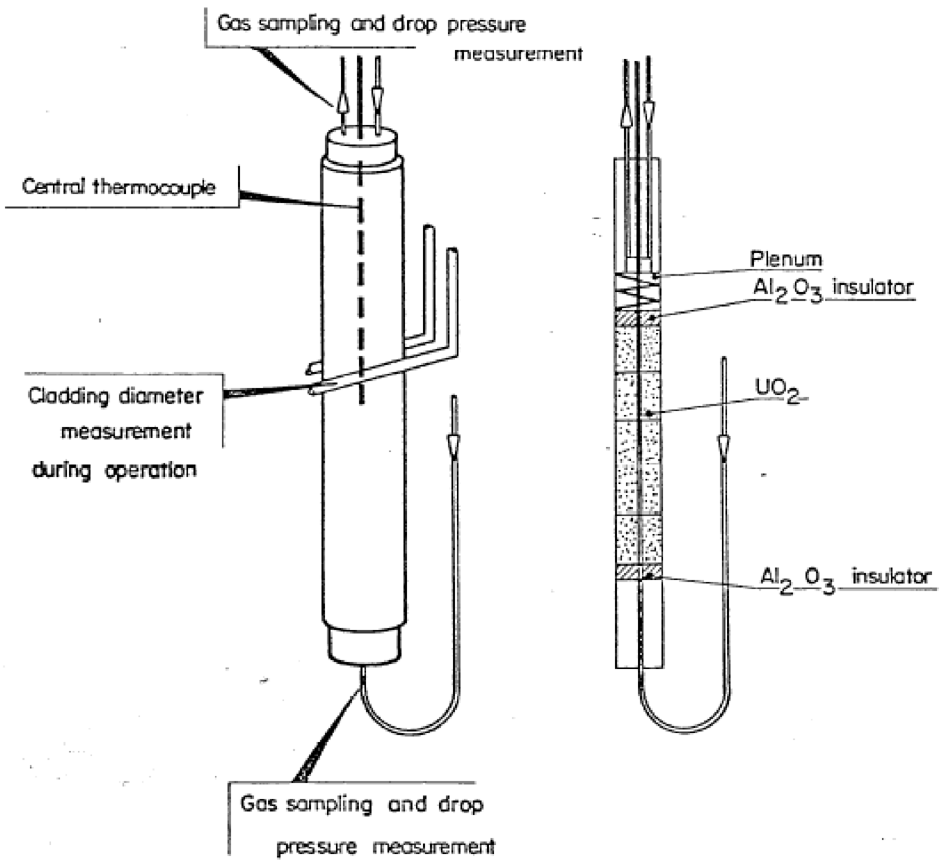
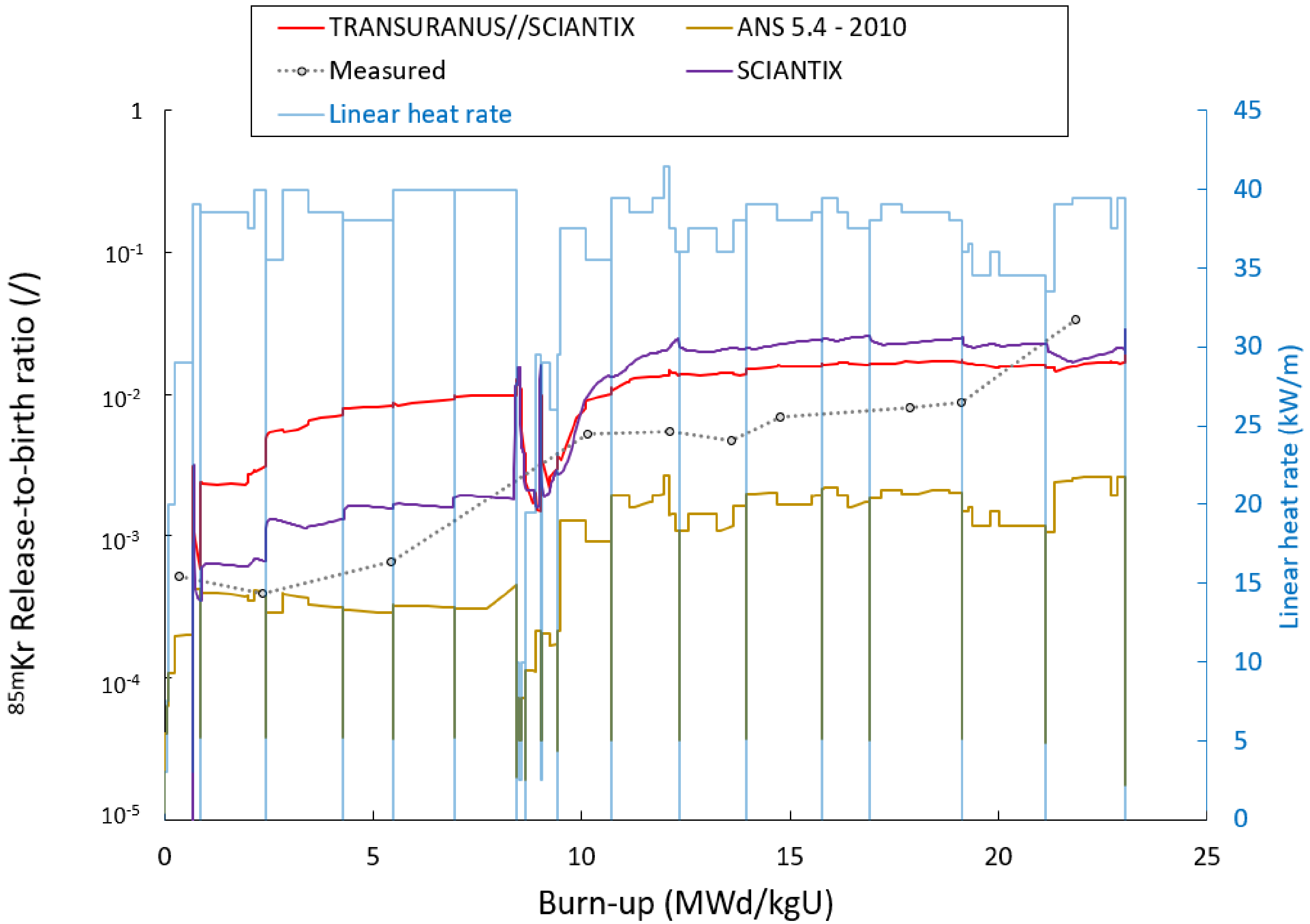


Fig.1 . EXPERIMENTAL FUEL ROD SCHEME

Unstable FGR from fuel in CONTACT experiment



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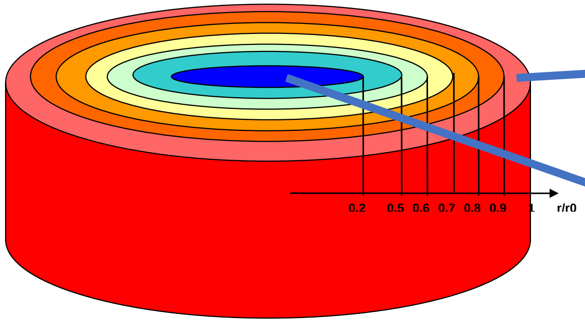
MFPR-F (IRSN)

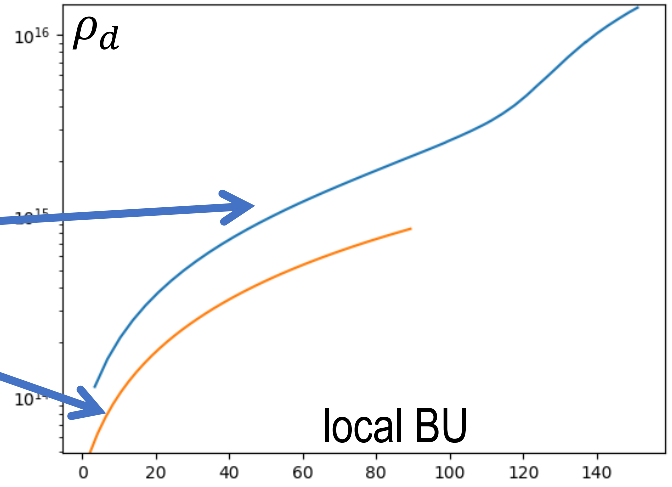
- Fuel rod behavior during LOCA transient
    - Formation of HBS zone
    - Fission Products release from HBS zone

- FP release from defective fuel rods with MFPR-F

The HBS formation

- The rim of the pellet: a cold and highly irradiated zone
  - ⟹ accumulation of dislocations
  - ⟹ important increase of disl. density ρ_d

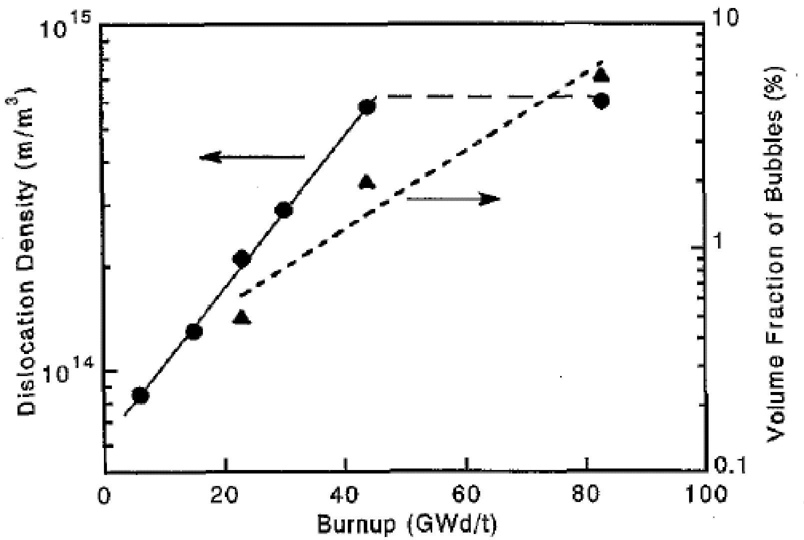




- Experimental data:

  HBS appears at $\rho_d \sim 10^{15}\ m^{-2}$

  - *Nogita & Une, Nucl. Instr. and Meth. in Phys. Research B 91 (1994) 301*

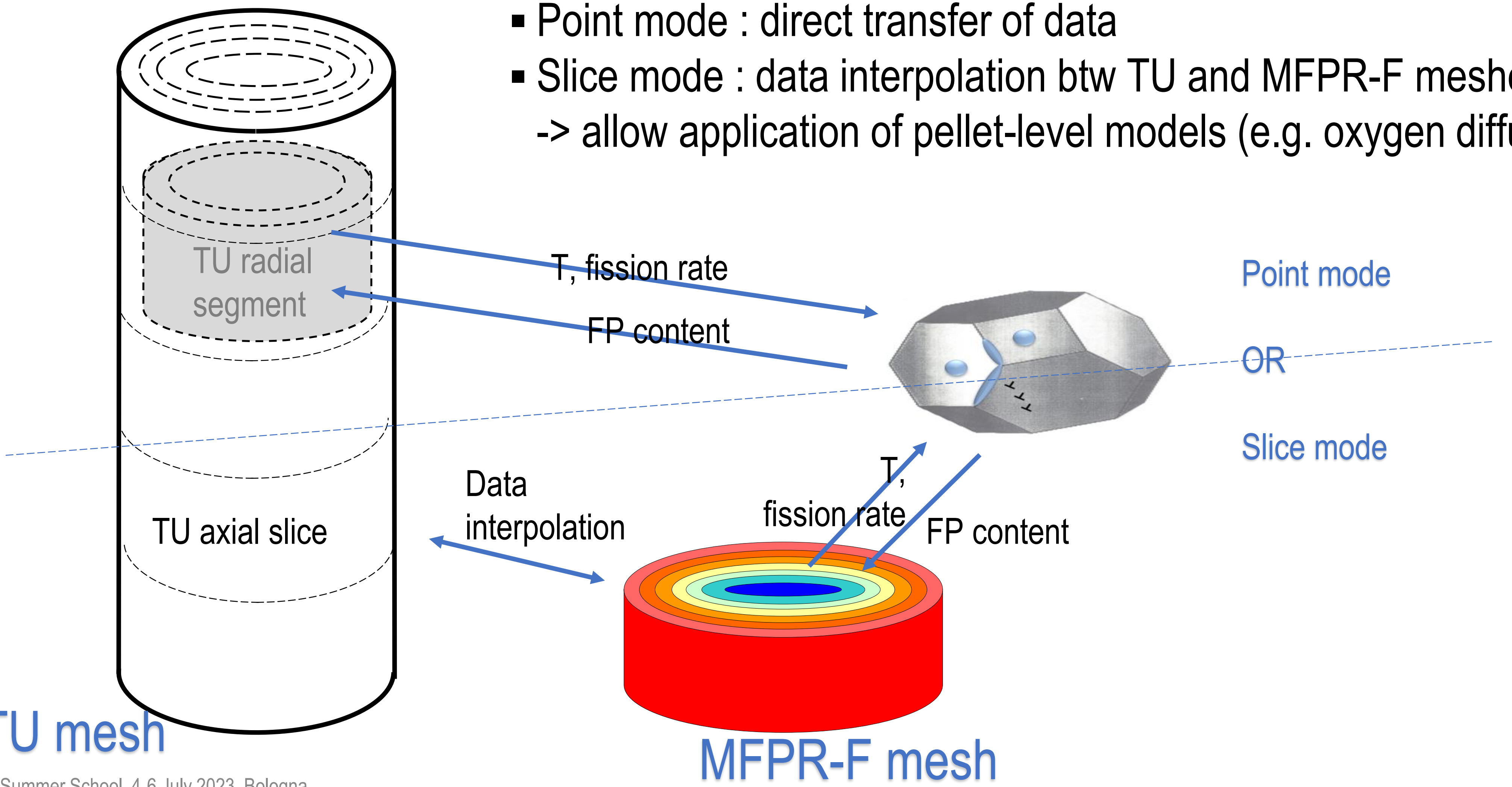


- HBS formation condition $\rho_d > \rho_d^{HBS}$

M.S. Veshchunov , V.E. Shestak, J. Nucl. Mat. 384 (2009) 12-18
F. Kremer, et al ", Proc. (TopFuel), 30 Sep – 4 Oct 2018, Prague, Czech Republic

Coupling of MFPR-F with TRANSURANUS

- Two modes of coupling:
  - Point mode : direct transfer of data
  - Slice mode : data interpolation btw TU and MFPR-F meshes
    -> allow application of pellet-level models (e.g. oxygen diffusion)



Assessing the formation of the HBS

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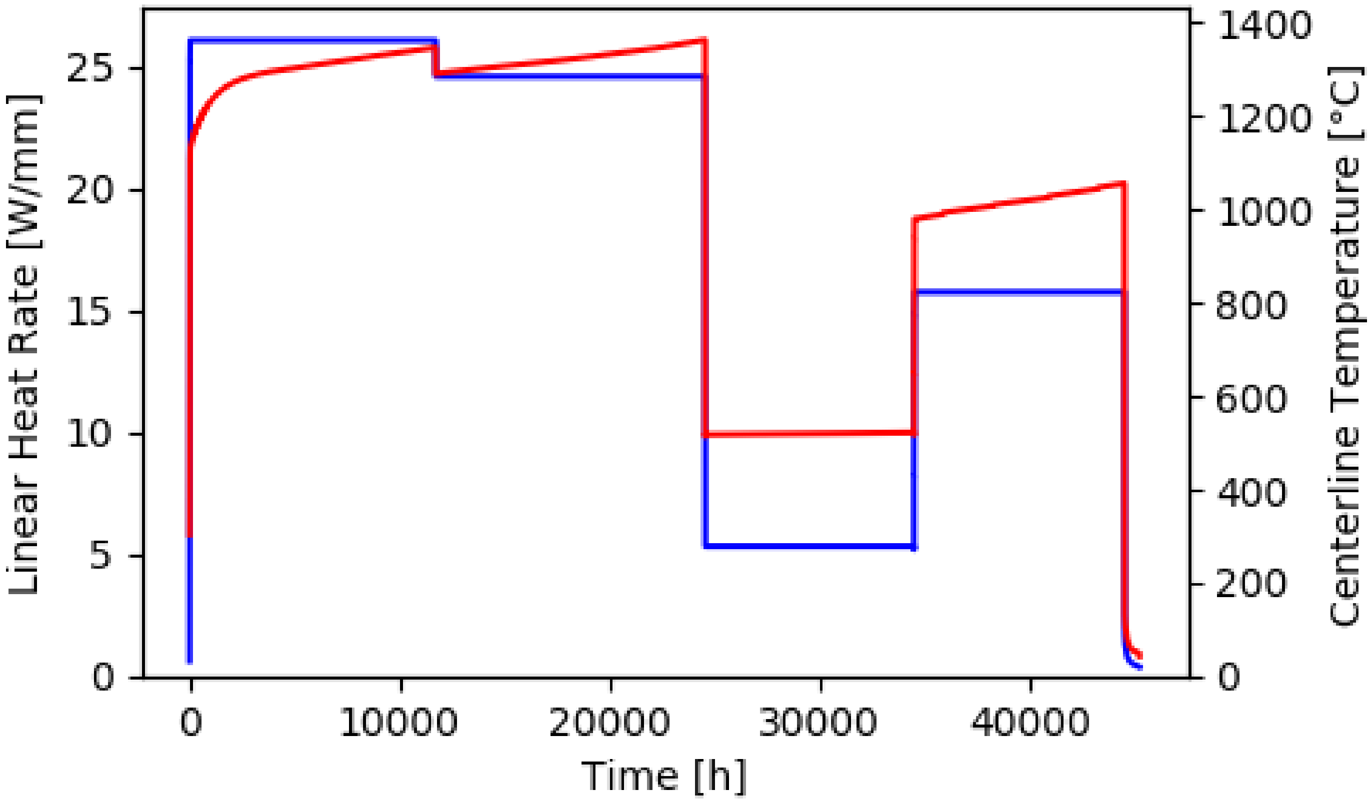
- **Application : Studsvik NRC192 case**
  - From IFPE database
  - Analyzed in IAEA FUMAC project

- **Irradiation 4 cycles**
  - Final burn-up 72 GWd/tU
  - Low power 3rd cycle

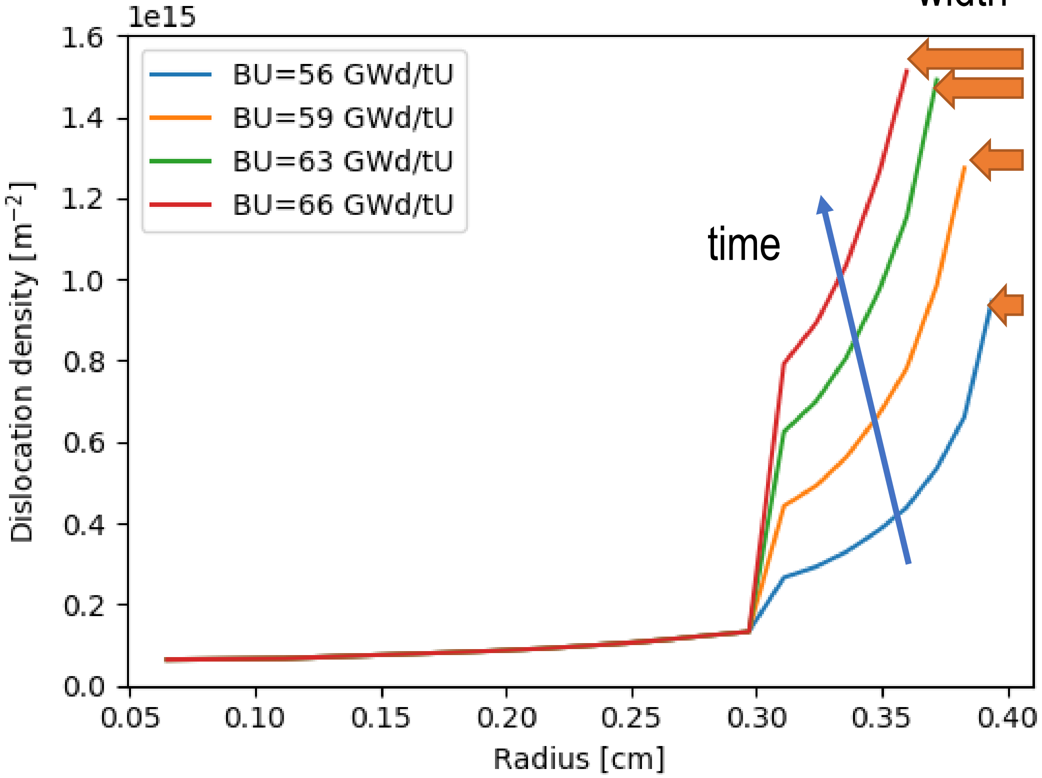


Formation of the HBS zone

- The pellet rim: cold and highly irradiated
  - accumulation of dislocations as expected

- HBS condition $\rho_d > \rho_d^{HBS}$
  - HBS zone extends progressively inside the pellet

HBS width



Fission product release from HBS zone

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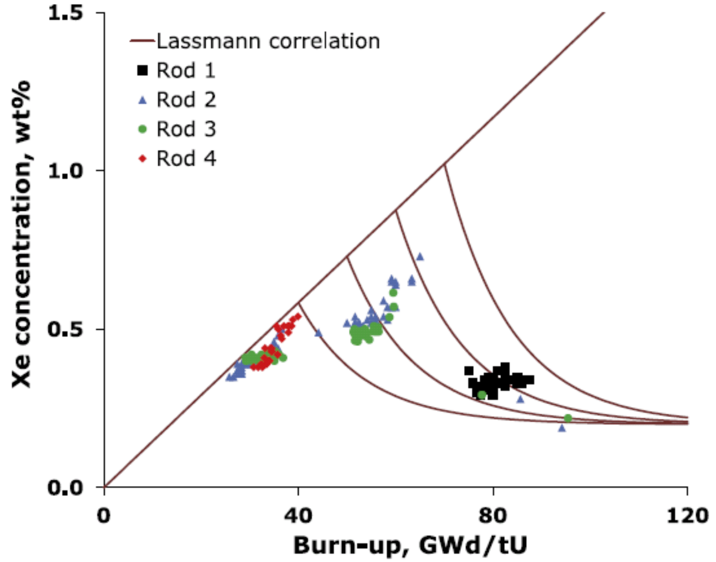
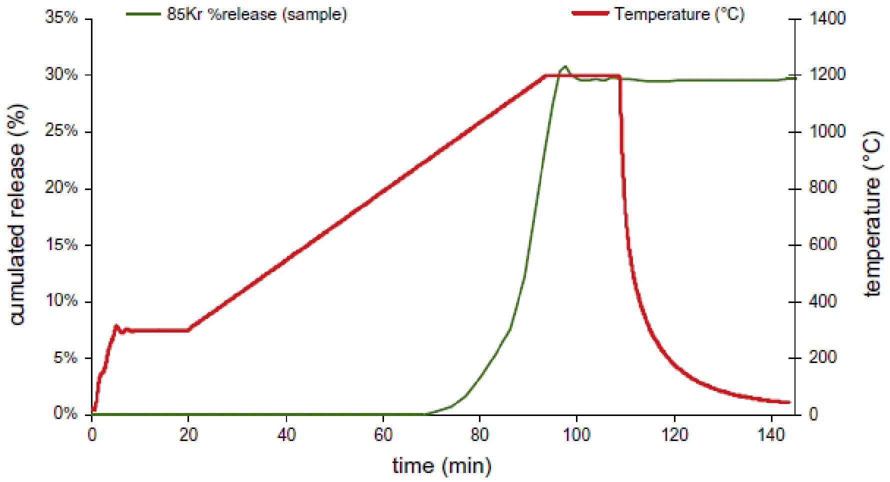
- During irradiation: grain depletion
  - FG and volatile FP migrate outside grain into huge HBS pores
  - No release from HBS pores

- During annealing : low-T release
  - Overpressurized pores
  - Burst release
  - Associated with fuel fragmentation

  - Hypothesis : pore overpressure responsible for FP/FG release





FP release from HBS zone: MFPR-F model

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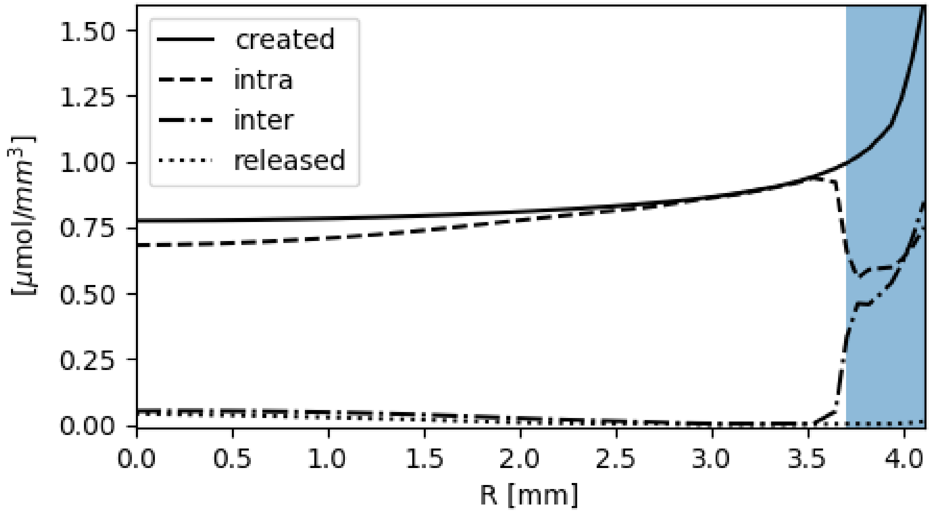
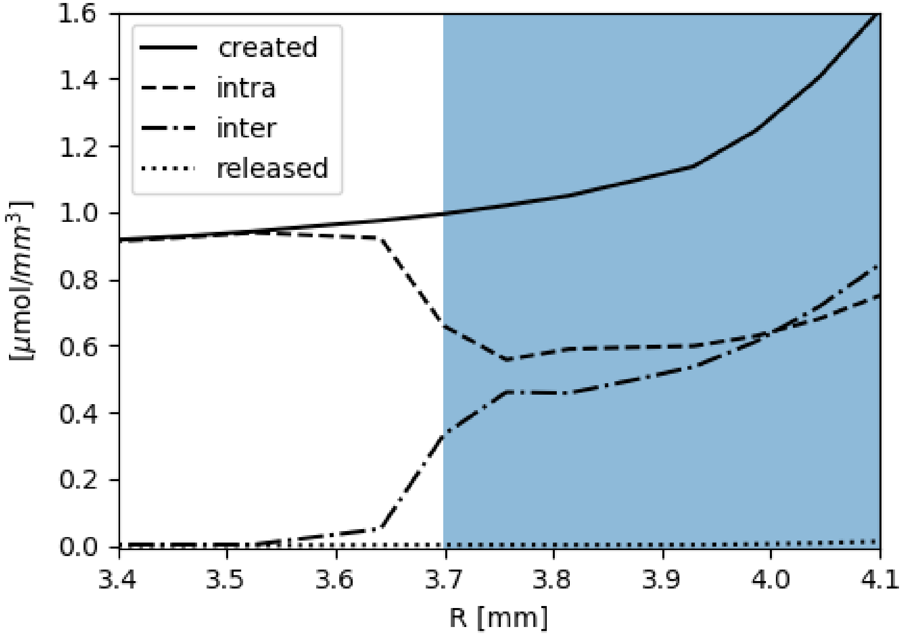
- Pressure condition for release
  - Pore internal pressure :
    $PV = NRTf(V,T)$ f : Equation of State
  - Release condition : $P > P_h + \Delta P_{crit}$
  - ΔP_{crit} pore overpressure

- Application to Studsvik LOCA case
  - Gas in HBS pores before LOCA transient :
    - 12% of total inventory
  - About 50% of FG in HBS zone is still inside the grain (probably underestimated)





Coupling of MFPR-F with TRANSURANUS

- Two modes of coupling :
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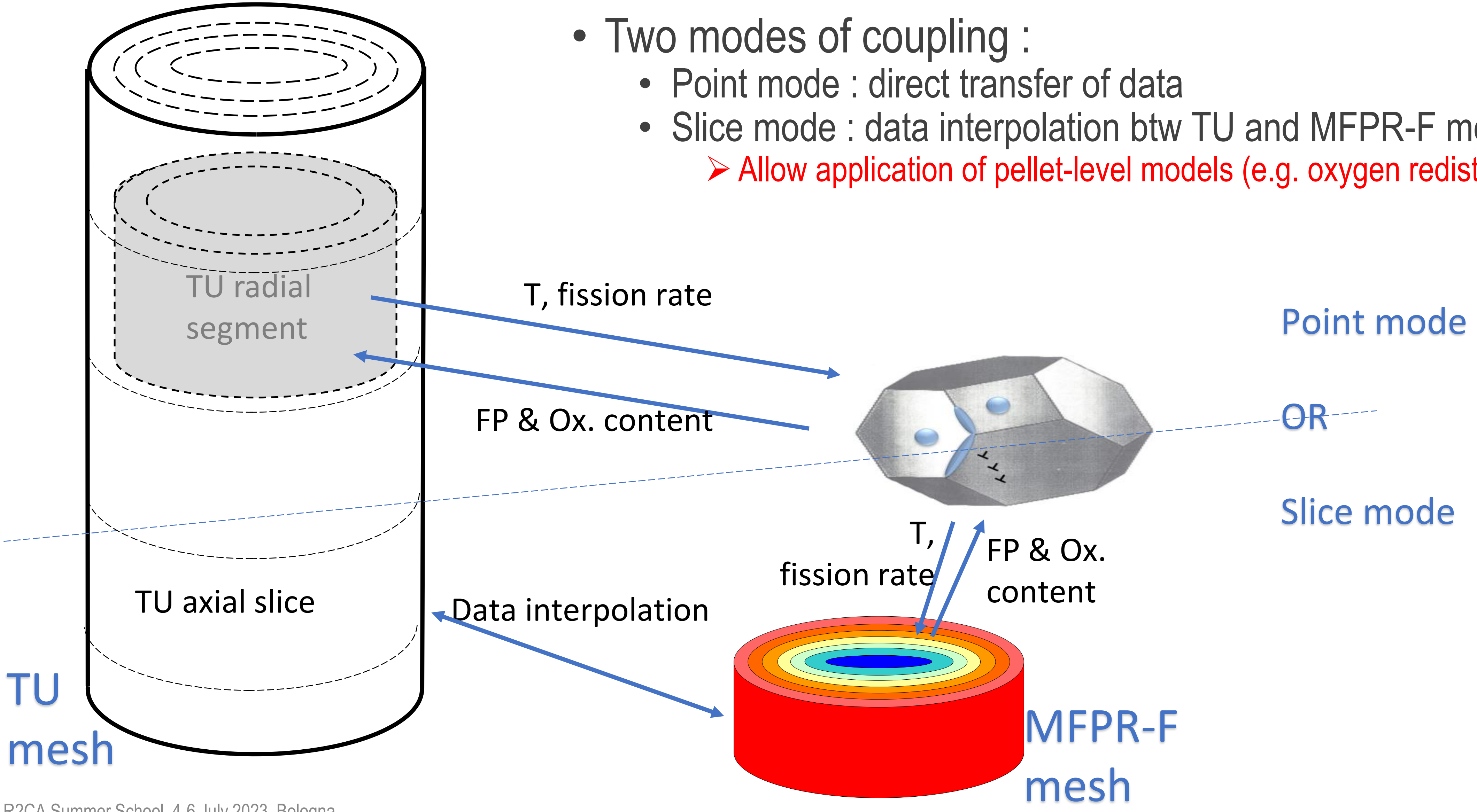
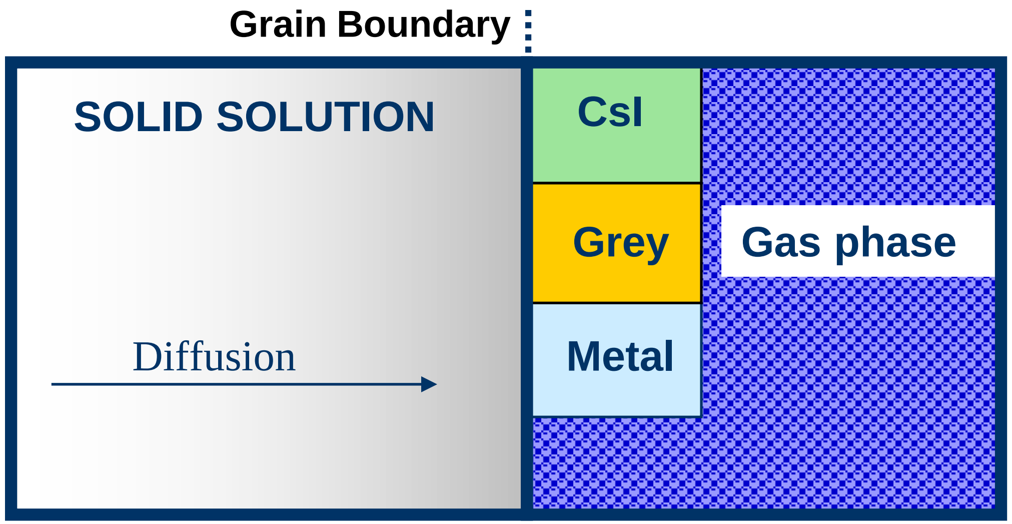


REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

System composition & basic processes (grain scale)

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- **Chemically active elements**
  Cs, Ce, I, Eu, Mo, Nd, Ru, Nb, Ba, Sb, Sr, Te, Zr, Xe, La
- **Principal phases**
  - UO_2-FP solid solution :
    - Cs
    - Ba, Sr and BaO, SrO
    - Zr, ZrO_2, Nb, NbO, NbO_2
    - La, Ce, Eu, Nd and their oxides
    - Sb and SbO
    - Mo, Ru and MoO_2, RuO_2
    - O
  - Metal phase : Mo and Ru
  - Grey phase (complex ternary compounds) :
    - $BaUO_4$, $SrUO_4$, Cs_2UO_4
    - $BaMoO_4$, $SrMoO_4$, Cs_2MoO_4
    - $BaZrO_3$, $SrZrO_3$, Cs_2ZrO_3
  - Separate solid phase : CsI
  - Gas phase : Xe, Te, I, Cs, CsI, Cs_2MoO_4, $(MoO_3)_{1-3}$, RuO_{1-4}, Ba_{1-2}, $(BaO)_{1-2}$, Sr_{1-2}, SrO, ZrO_{1-2}, LaO, CeO, NdO, NbO, O_2 …



Transport equation in solid solution

$$\frac{\partial Y_i}{\partial t} = B_i + \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_i r^2 \frac{\partial Y_i}{\partial r}\right)$$

Boundary conditions:
thermo-chemical equilibrium between various phases on GB

Release: subsequent migration of FP elements in the form of gaseous compounds to open porosity

Oxygen redistribution in MFPR-F

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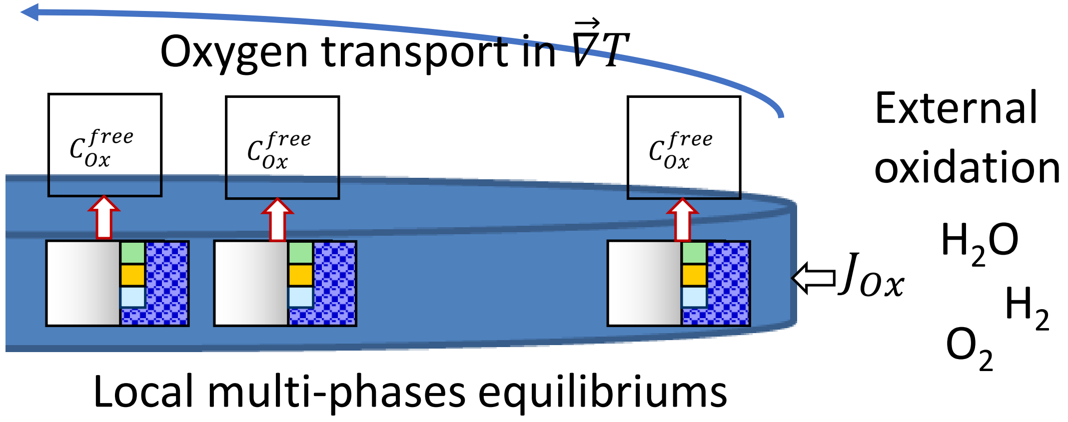
- Oxygen diffusion at **the pellet scale**
  - J : diffusion flux
  - S : source (ox. liberated by fission) and sink (ox. lost by oxides FP release)

$$\frac{\partial}{\partial t}\overline{C}_{Ox}^{(tot)} = -\frac{1}{r}\frac{\partial}{\partial r} rJ + S(r,t)$$

- Diffusion flux driven by gradients of :
  - Local concentration of dissolved « free » oxygen
    - ➢ Driven by local multi-phases equilibriums
  - Temperature (Soret effect)

$$-J = D\frac{\partial C_{Ox}^{(free)}}{\partial r} + DC_{UO_2}\chi\frac{\partial T}{\partial r}$$

- Boundary condition : external oxygen flux J_{Ox}
  - Normal operations : $J_{Ox} = 0$
  - Off-normal operations (clad rupture) : fuel surface oxidation by (user-defined) surrounding atmosphere $J_{Ox} = f(P_{H_2O}, P_{H_2}, P_{O_2})$



→Towards simulation of defective fuel rods

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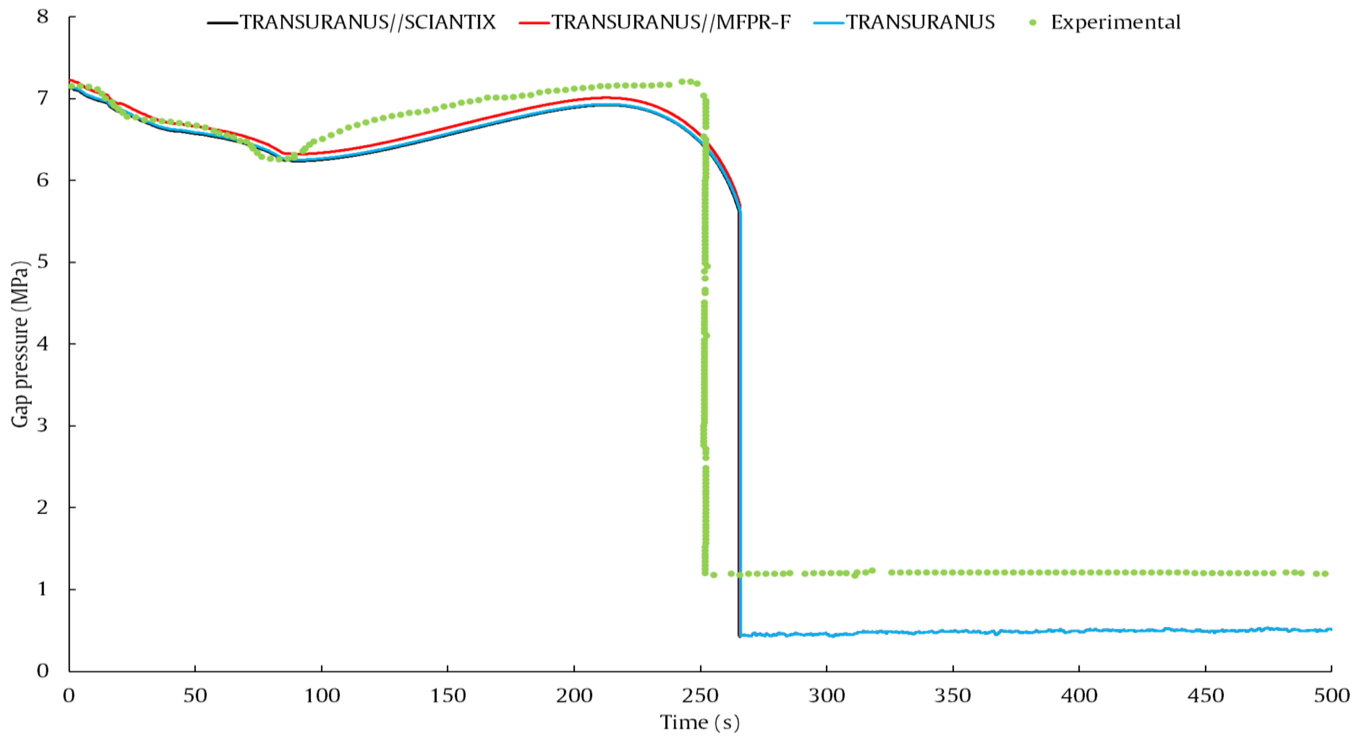
LOCA modelling of fission product behavior with coupled codes

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Coupling TRANSURANUS (Fortran) and mechanistic meso-scale modules for fission product behaviour SCIANTIX (C++) and MFPR-F (Fortran)

- Database has been identified
  - IFA-650.10
  - IFA-650.11
  - Studsvik-192

- Coupling successful without convergence or cliff-edge effects.



Outline of developments for TRANSURANUS and FRAPCON

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- H uptake during LOCA (NucleoCon)
- Upgraded LOCA models: effect of H on phase transition, creep, burst stress (PreussenElektra/TUMünchen) for Zry and M5 (ENEA)

See previous presentation by Tatiana Taurines

- Radioactive FP release
  - ANS5.4 model for radioactive FP release (FORTUM)
  - Radioactive FP release in SCIANTIX-TRANSURANUS (POLIMI)
  - Radioactive FP release from defective rods (NINE)
- Coupling TRANSURANUS with meso-scale models SCIANTIX, MFPR-F
- Hydrogen redistribution (CIAE, KL), coupling with HYDCLAD model of CIEMAT
- Implement new ATF properties (IPEN, INRNE, NINE, NFQ, CIEMAT, UCAM)
- Axial migration in gap (before/after defect formation) (UJV)

Radioactive FP release from defective rods

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

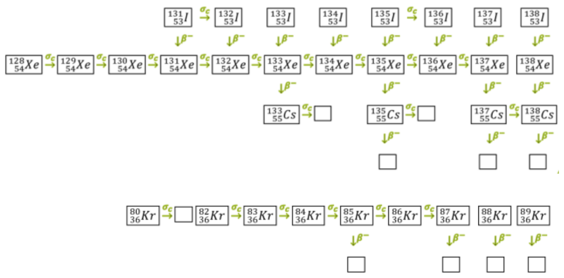
- Activities of L. Giaccardi, now PhD at UNIPI
  - Implementation of model for FGR from defective fuel rods
  - Improvements in TRANSURANUS (graded approach)
    1. Production of a large number of isotopes of most important FP species
    2. FGR from fuel to gap, and from gap to coolant of all the isotopes considered
    3. Calibration of FGR model from defective rod
    4. Verification and Validation

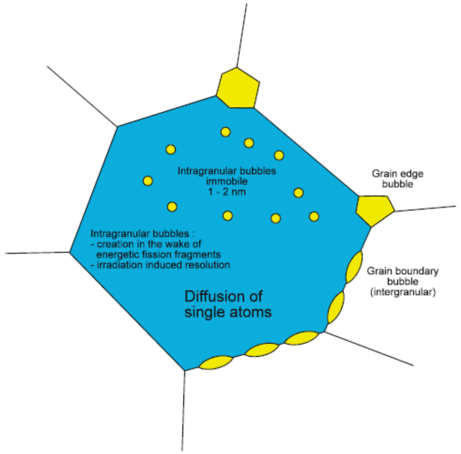
FGR Model from Defective Rods

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

FUEL | **GAP** | **COOLANT**

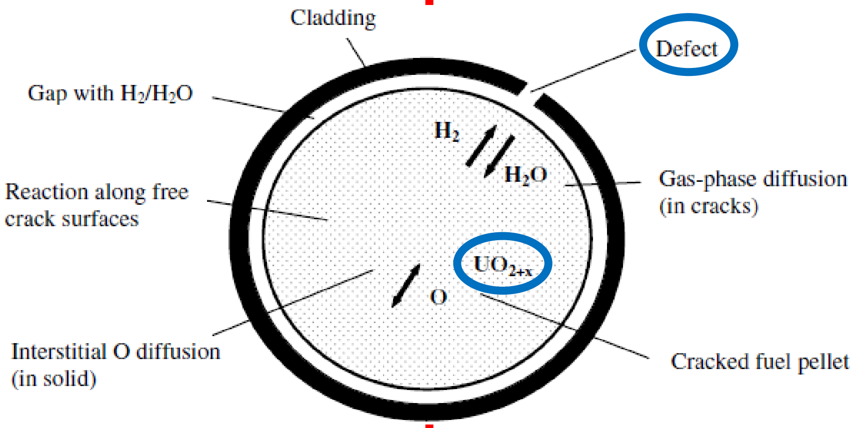
Isotopes Production
Xe, Kr, Cs, I





Isotopes Diffusion in the Fuel

Isotopes Accumulation at the Grain Boundaries



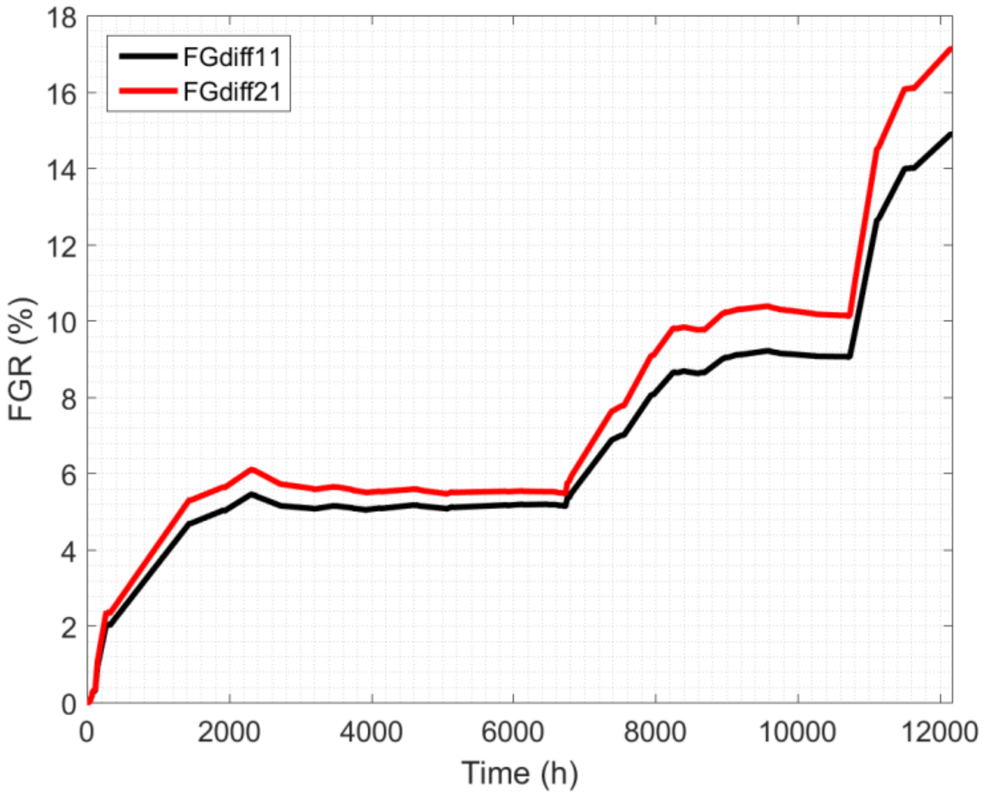
FGR from Fuel to Gap

FGR from Gap to Coolant

Fuel behaviour with TRANSURANUS in defective fuel rods

Collaboration between **POLIMI** and **NINE** is ongoing to harmonize common models and routines in TRANSURANUS for fission product behaviour.

- Modelling of FP release to the gap by NINE, including fuel oxidation by coolant through an effective diffusivity.
- Ongoing activities on gap-to-coolant release of short-lived FP, based on open literature model for defective rods during stationary operation.
  - Validation with CRUSIFON experiments (IFPE public database).



Impact of the fuel stoichiometry deviation on the FG release, due to the increase of the gas diffusivity.

Perspectives of defective fuel simulation with TRANSURANUS

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Extend preliminary model for FGR from defective fuel rods
  - FGR from fuel to gap
  - Empirical model to estimate release rate from defective cladding to coolant
- V&V Activities
- Coupling with TH codes to simulate gap pressure evolution of defective fuel rods (i.e. water evaporation and steam condensation inside the gap, the partial pressures evolution, and finally the non-condensable release from the gap into the coolant) → transient cases

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H-redistribution and hydride formation

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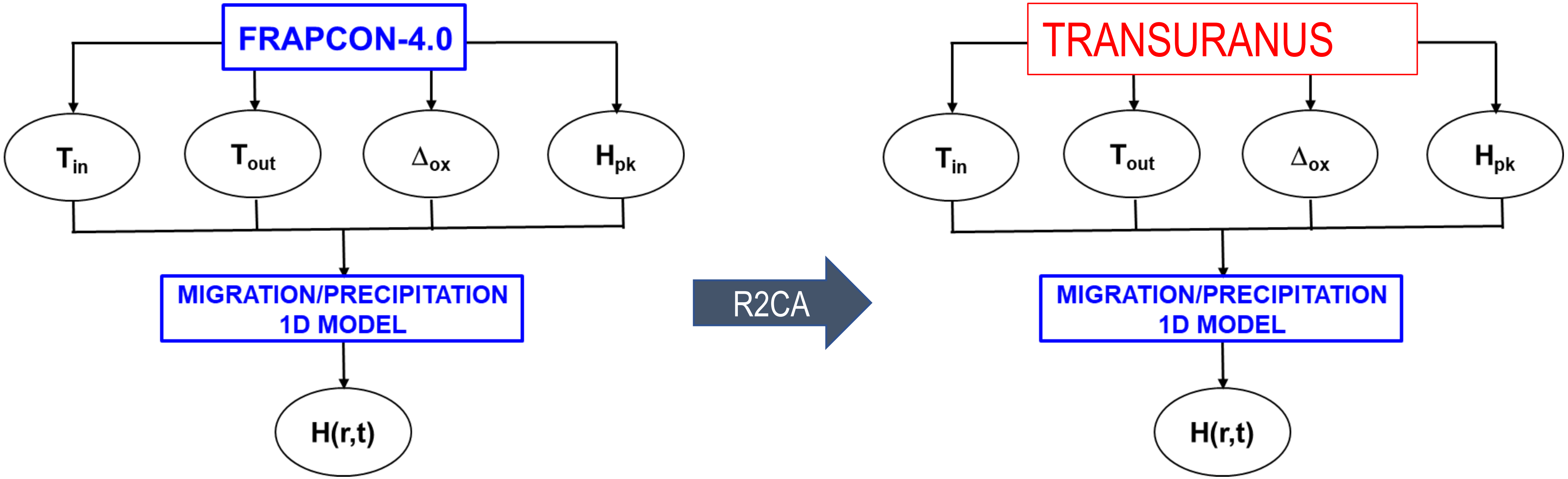
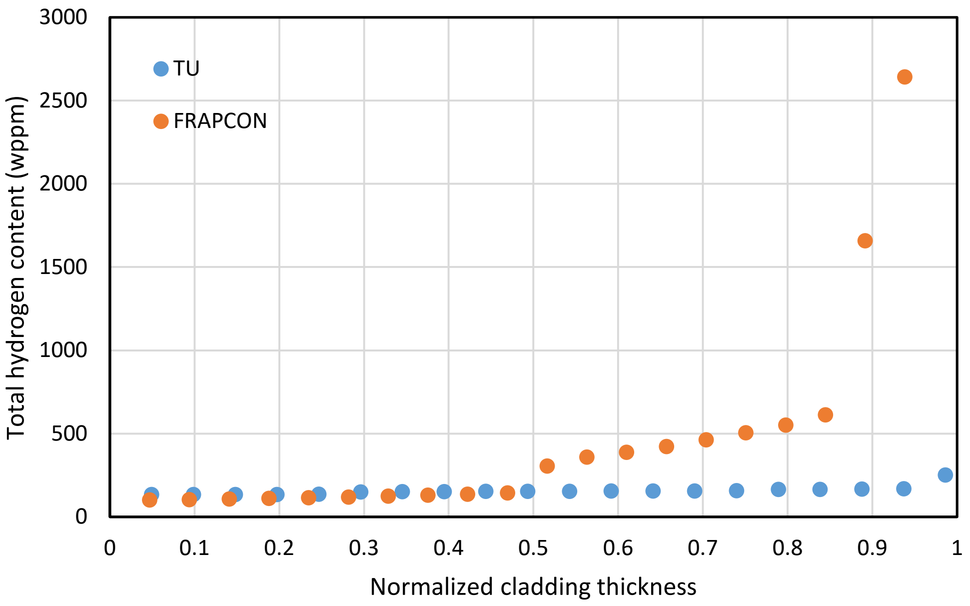
- HYREDI1, HYREDI2: standalone, only hydride redistribution (no precipitation) based on diffusion and Soret effect
- CIEMAT´s in-clad hydrogen migration/precipitation model coupled with the fuel performance code FRAPCON-4.0 (JNM: Feria and Herranz, 2018) updated with new precipitation model from BISON (JNM: Passelaigue et al., 2021)



First results of coupling HYDLAD with TRANSURANUS and comparison with FRAPCON on basis of base irradiation of IFA650.10

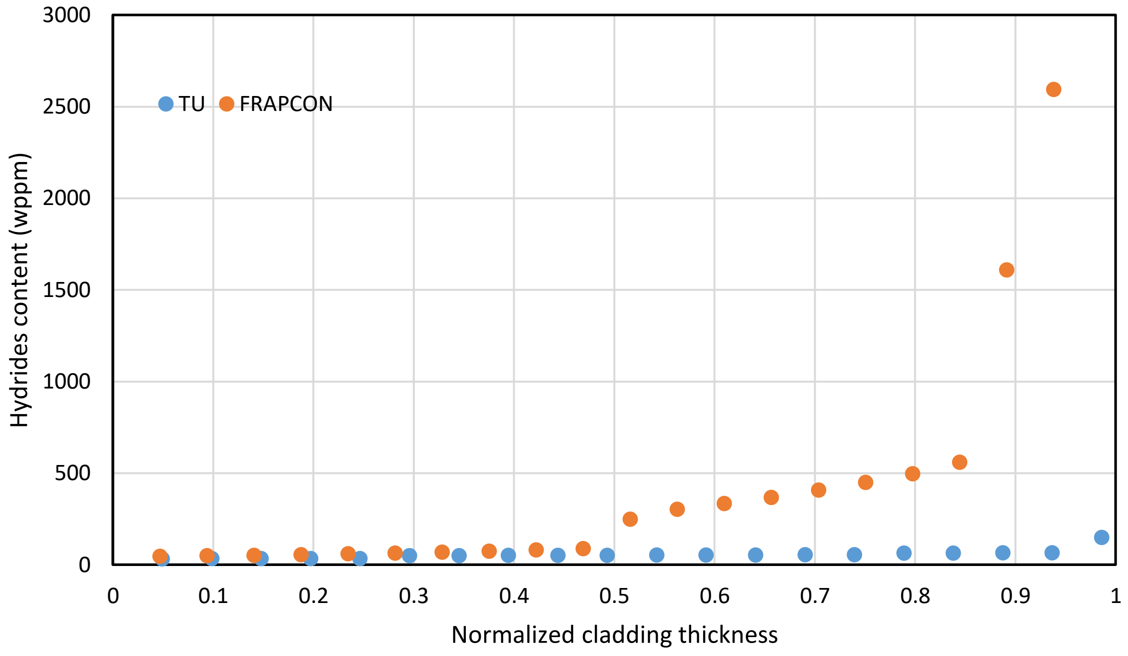


Total hydrogen content as a function of the normalized cladding thickness at EOL

Encouraging preliminary first results

Visiting PhD:
Pau Aragon (CIEMAT)

Hydrides content as a function of the normalized cladding thickness at EOL.



ATF properties included in TRANSURANUS

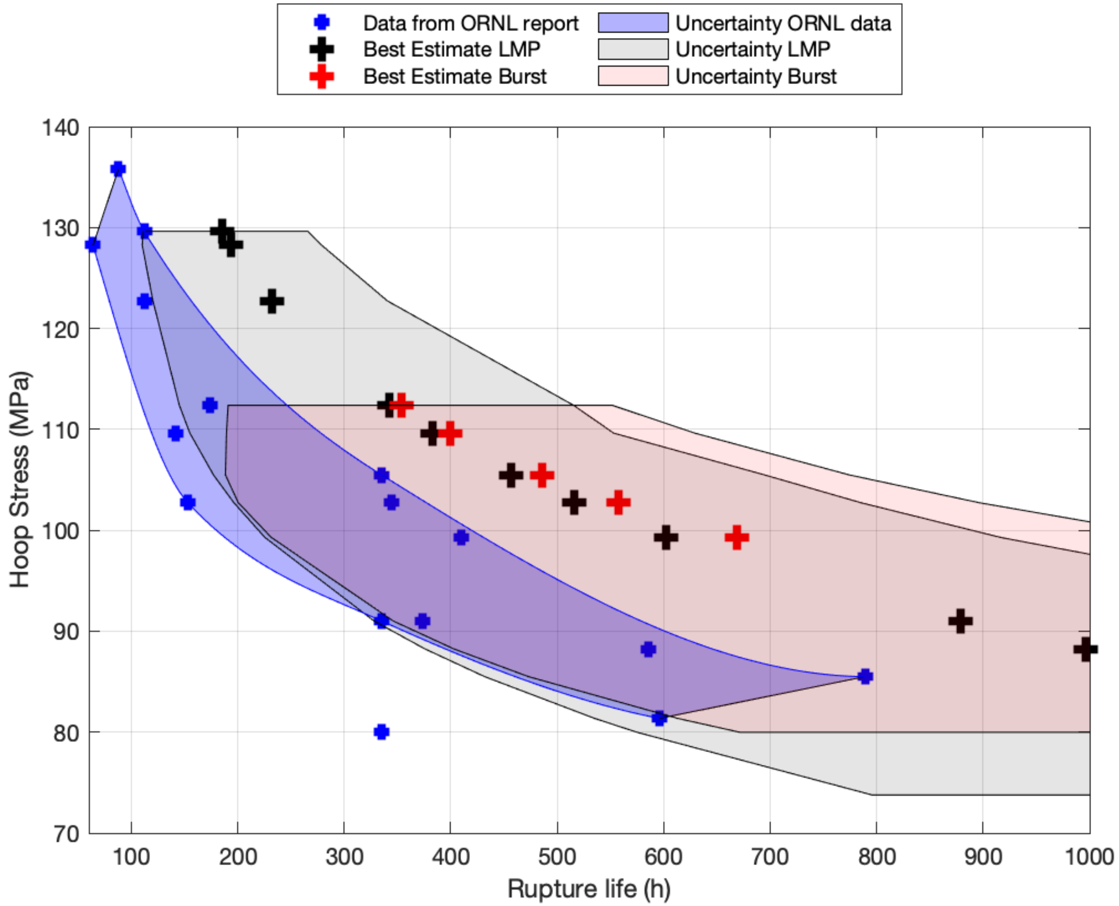
- Fuels
  - ✓UN
  - ✓U_3Si_2
  - Cr-doped UO_2

- Claddings
  - ✓SS
  - ✓FeCrAl
  - ✓Cr-coated Zry
  - Hastelloy

First integral assessment of Hastelloy with burst tests from ORNL

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- New material properties and models for Hastelloy and FLiBe coolant implemented in TRANSURANUS fuel performance code for preliminary design calculations of a new Molten Salt Reactor
- For each required property of the Hastelloy cladding, an independent set of data was applied for validation whenever possible
- An preliminary uncertainty and sensitivity analysis by means of TUPython was also carried out, enabling to better steer future experimental work
- A first integral TRANSURANUS code assessment for Hastelloy was based on simulation of burst tests carried out at ORNL



A. de Lara et al (UCAM), submitted to ANE

UNIVERSITY OF CAMBRIDGE

Collaboration with CIEMAT

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Comparison FRAPTRAN – TRANSURANUS for LOCA
- The TUmech stand-alone
- Modelling FeCrAl ATF cladding
- A modified treatment of plasticity
- Coupling TRANSURANUS with HYDCLAD

Visiting PhD:
Pau Aragon (CIEMAT)

Application of standalone TUMECH

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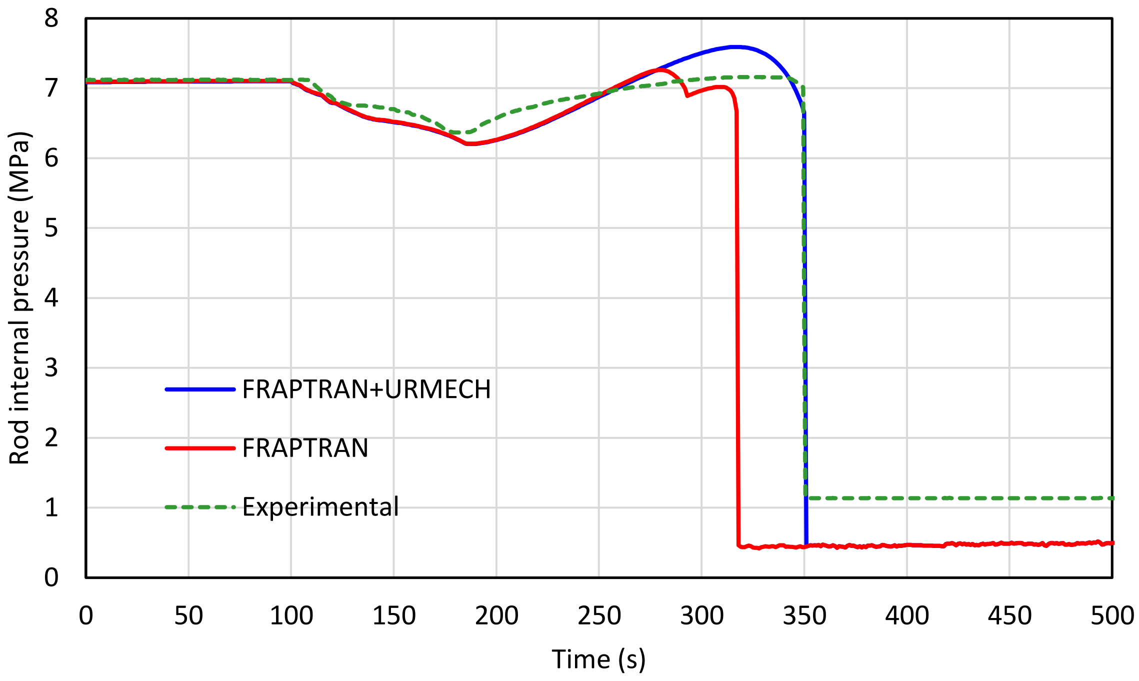
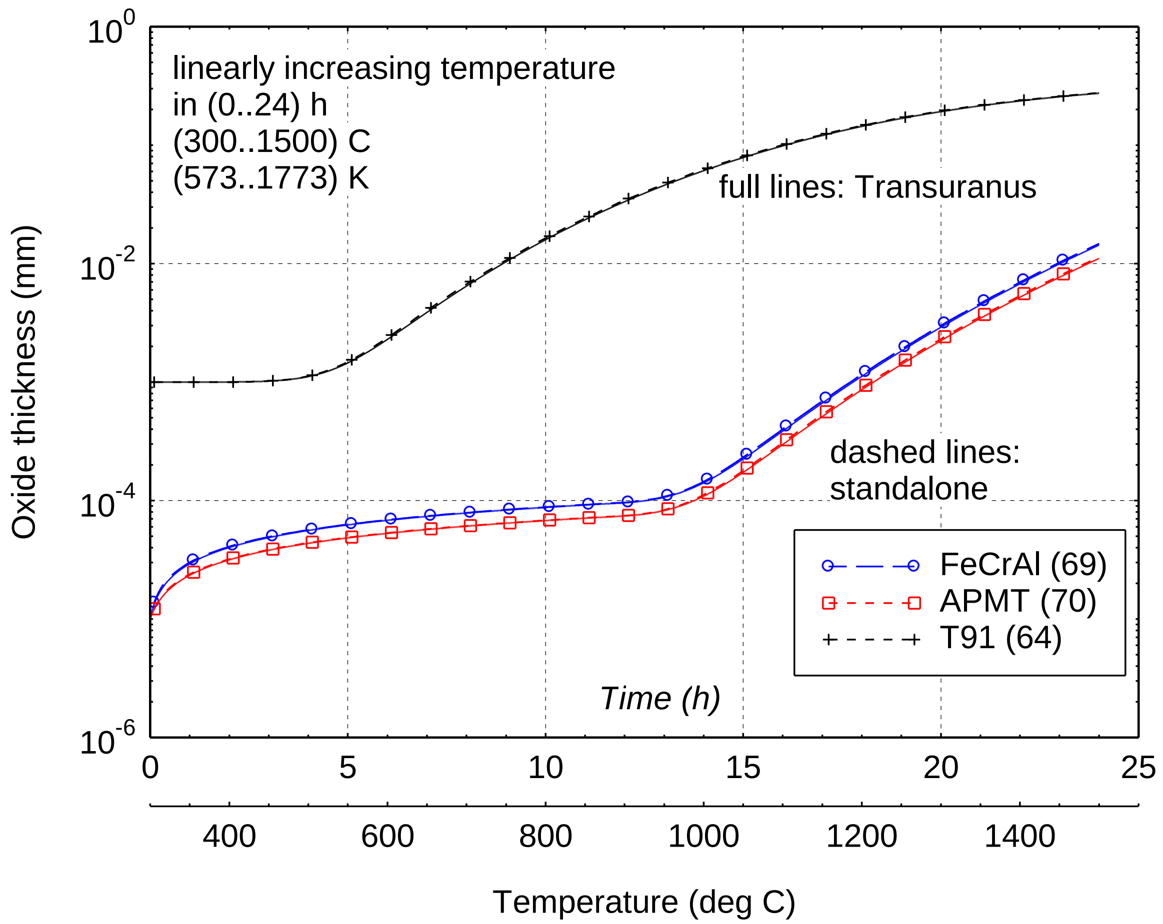
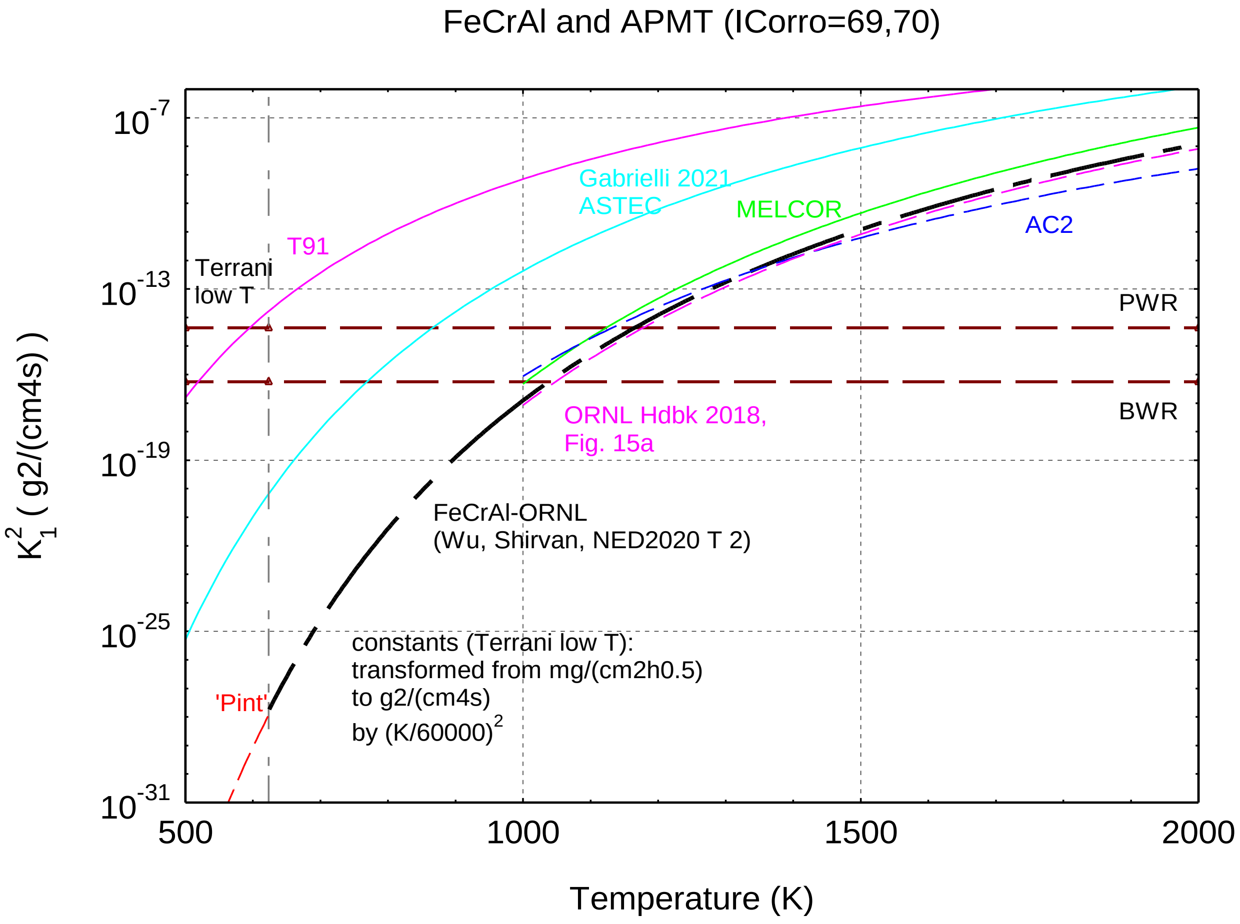
Visiting PhD:
Pau Aragon

- May be implemented in other fuel performance codes as an alternative mechanical model
- Halden LOCA test IFA-650.10 simulated using FRAPTRAN + TUmech



Implementing High-T corrosion for FeCrAl in TRANSURANUS





This project has received funding from the Euratom research and training programme 2019-2020 under grant agreement No 945063.

European Commission

FUMEX-II case considered (see PBCN2022)

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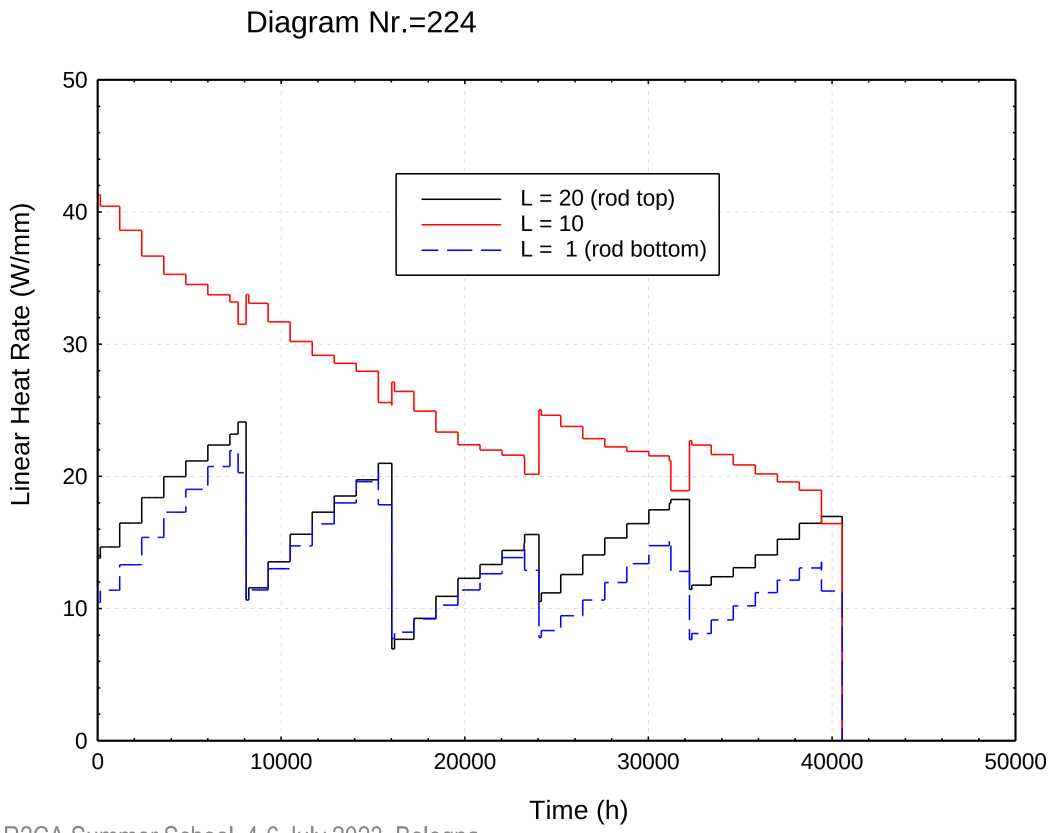
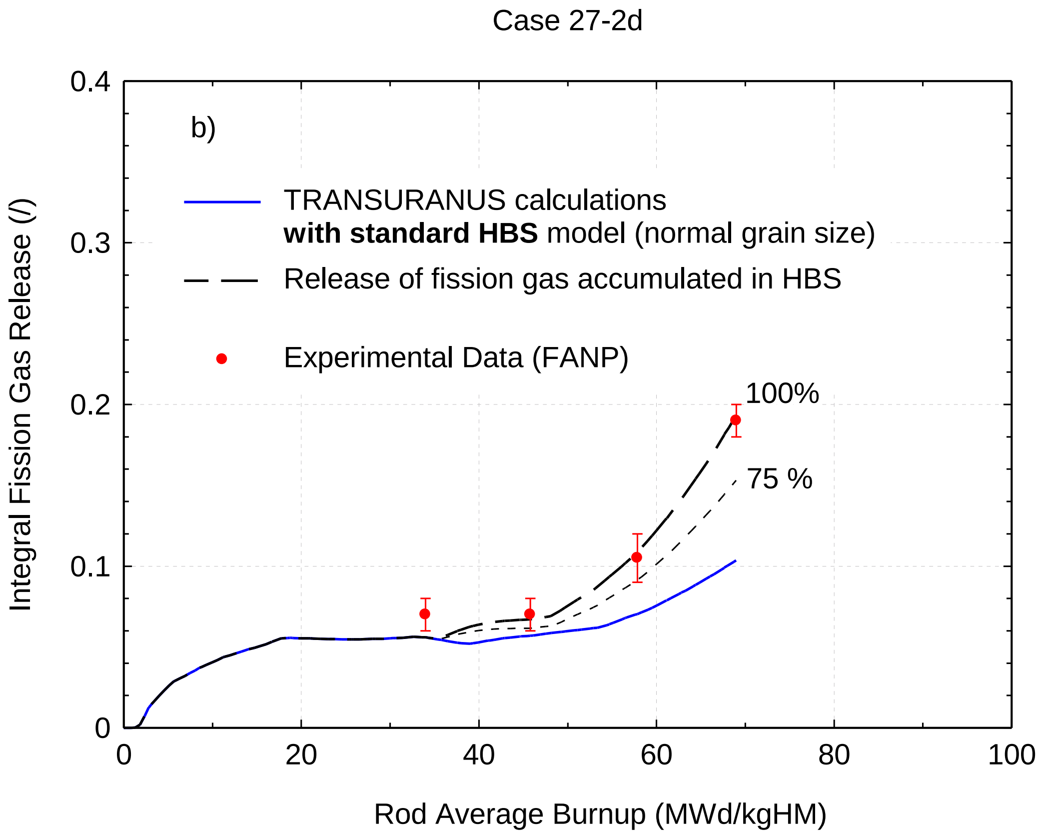
Assessment of TRANSURANUS:

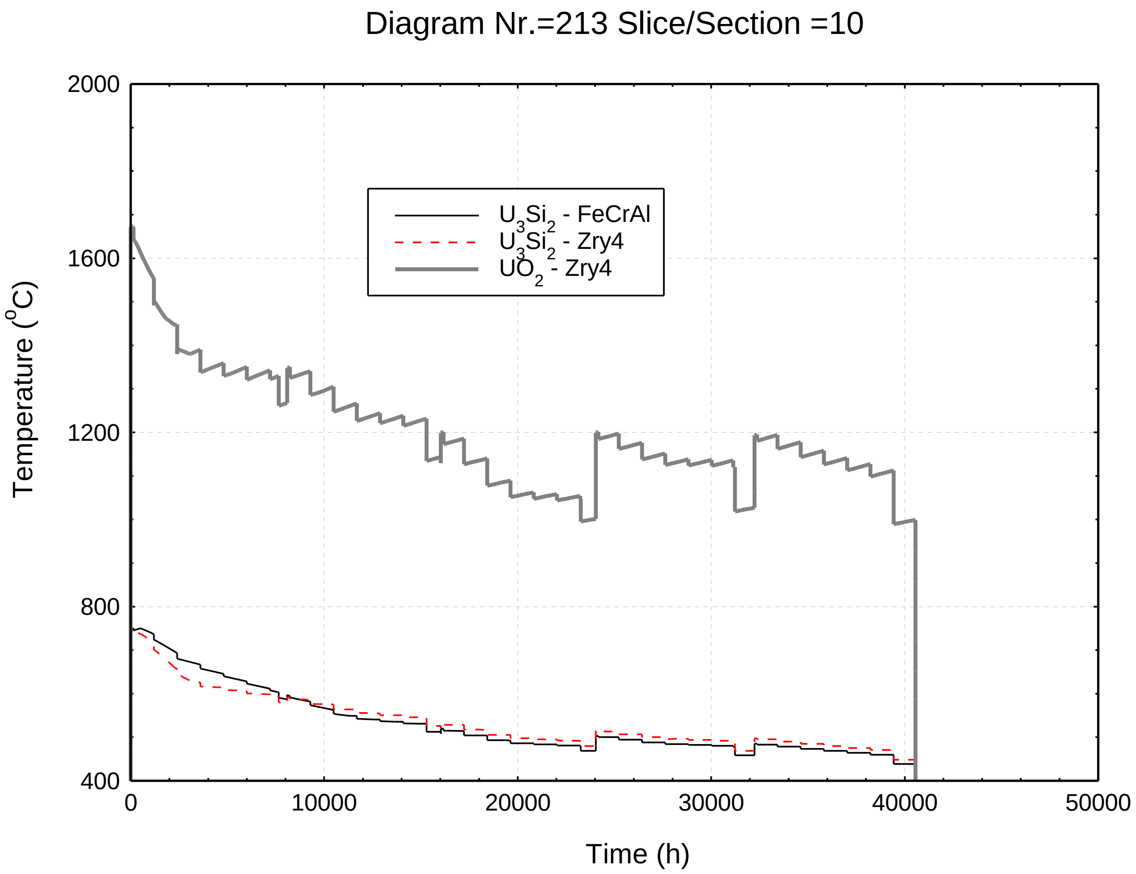
- Case 27 provided by Framatome
- PWR rod with Zry4 cladding

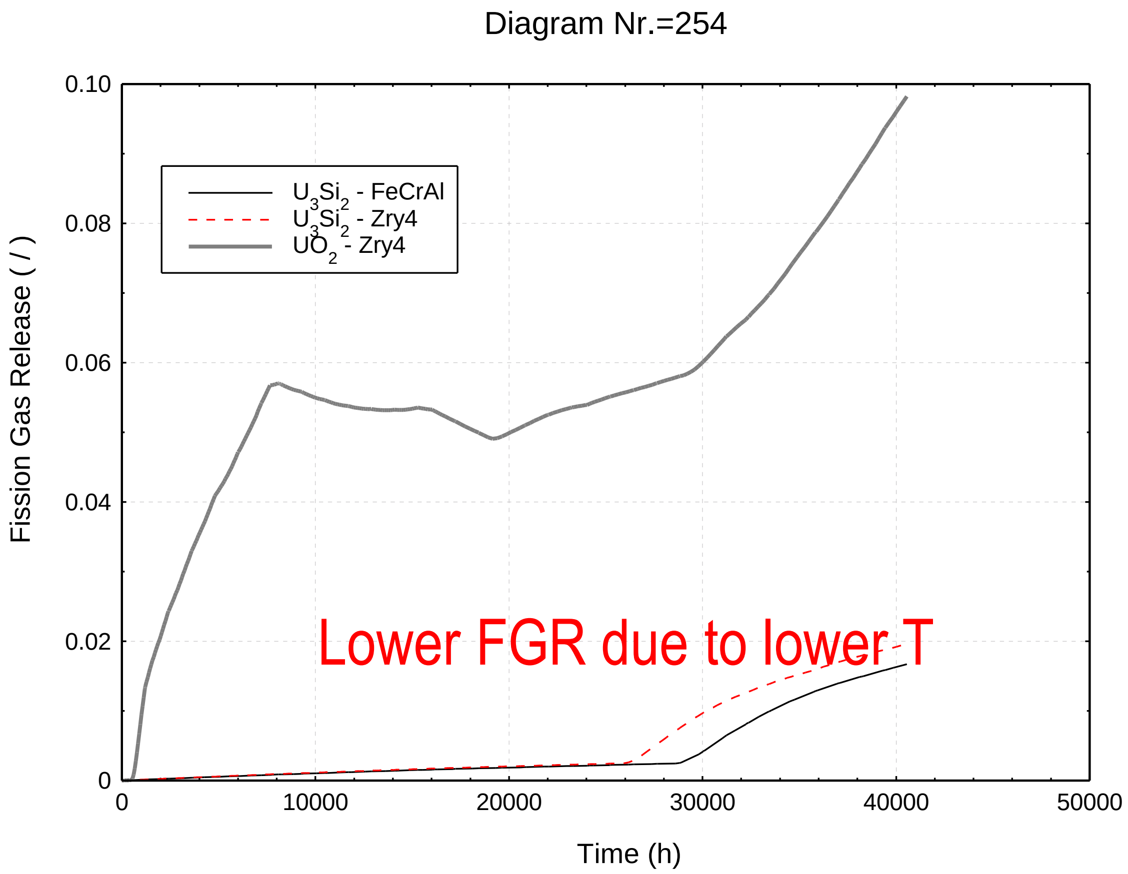




Impact of ATF on central T and FGR

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS





Summary of main fuel model developments

- More mechanistic modelling of fission gas behavior
  - Coupling SCIANTIX and MFPR-F with TRANSURANUS, FRAPCON
- Extension to radioactive fission product release
  - TRANSURANUS
  - SCIANTIX: implementation of ANS5.4
- Extension to defective fuel modelling for TRANSURANUS
  - First model for release from defective model
  - Consideration of radial distribution of oxidation
- Inclusion of H redistribution, hydride formation
  - HYREDI1/HYREDI2 (TRANSURANUS), HYDCLAD
  - H-uptake for secondary hydride formation
- Stand-alone model for axial gas migration for coupling with TRANSURANUS
- Stand-alone model for clad mechanics for coupling with FRAPTRAN
- Inclusion of ATF properties (see next presentation of Eduard Pouiller)

List of publications

- G. Zullo, D. Pizzocri, L. Luzzi, «On the use of spectral algorithms for the prediction of short-lived volatile fission product release: Methodology for bounding numerical error", Nuclear Engineering and Technology, 54 (2022), 1195-1205
- G. Zullo, D. Pizzocri, A. Magni, P. Van Uffelen, A. Schubert, L. Luzzi, "Towards grain-scale modelling of the release of radioactive fission gas from oxide fuel. Part I: SCIANTIX", Nuclear Engineering and Technology 54 (2022) 2771-2782
- G. Zullo, D. Pizzocri, A. Magni, P. Van Uffelen, A. Schubert, L. Luzzi, "Towards grain-scale modelling of the release of radioactive fission gases from oxide fuel. Part II: coupling SCIANTIX with TRANSURANUS", Nuclear Engineering and Technology 54 (2022) 4460-4473
- G. Zullo, D. Pizzocri, L. Luzzi, F. Kremer, R. Dubourg, A. Schubert, P. Van Uffelen, "Towards simulations of fuel rod behaviour during severe accidents by coupling TRANSURANUS with SCIANTIX and MFPR-F", Annals of Nuclear Energy 190 (2023) 109891
- P. Van Uffelen, A. Schubert, Z. Soti, "Assessing the effect of some ATF materials and uncertainties on their properties under normal operation conditions by means of the TRANSURANUS code", Proc. of 23rd Pacific Basin Nuclear Conference, Volume 3, SPPHY 285, pp. 1-15, 2023
- F. Feria, L.E: Herranz, "Assessment of hydride precipitation modelling across fuel cladding: Hydriding in non-defective and defective fuel rods", Annals of Nuclear Energy, 188 (2023) 109810
- P. Aragón, F. Feria, L.E. Herranz, "Progress on modelling the thermo-mechanical performance of accident-tolerant fuels", Proc. The 2023 Water Reactor Fuel Performance Meeting (WRFPM2023), Xi'an, China, July 17-21, 202

Thank you!

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