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Multi-scale approach to advanced fuel modelling for enhanced safety

Summary

- Fuel rod modeling tools for safety analysis
- Example 1 : Intragranular fission gas bubble study
- Example 2 : Integral analysis of HBU fuel behaviour in LOCA
- Conclusion

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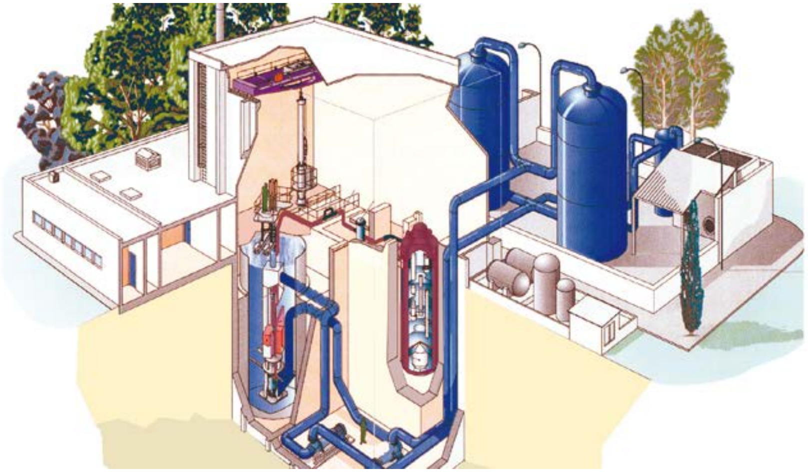
Fuel rod modeling tools for safety analysis

- To be able to analyze and predict fuel rod behavior :
  - Accident conditions
  - Normal conditions
  - Transport and storage

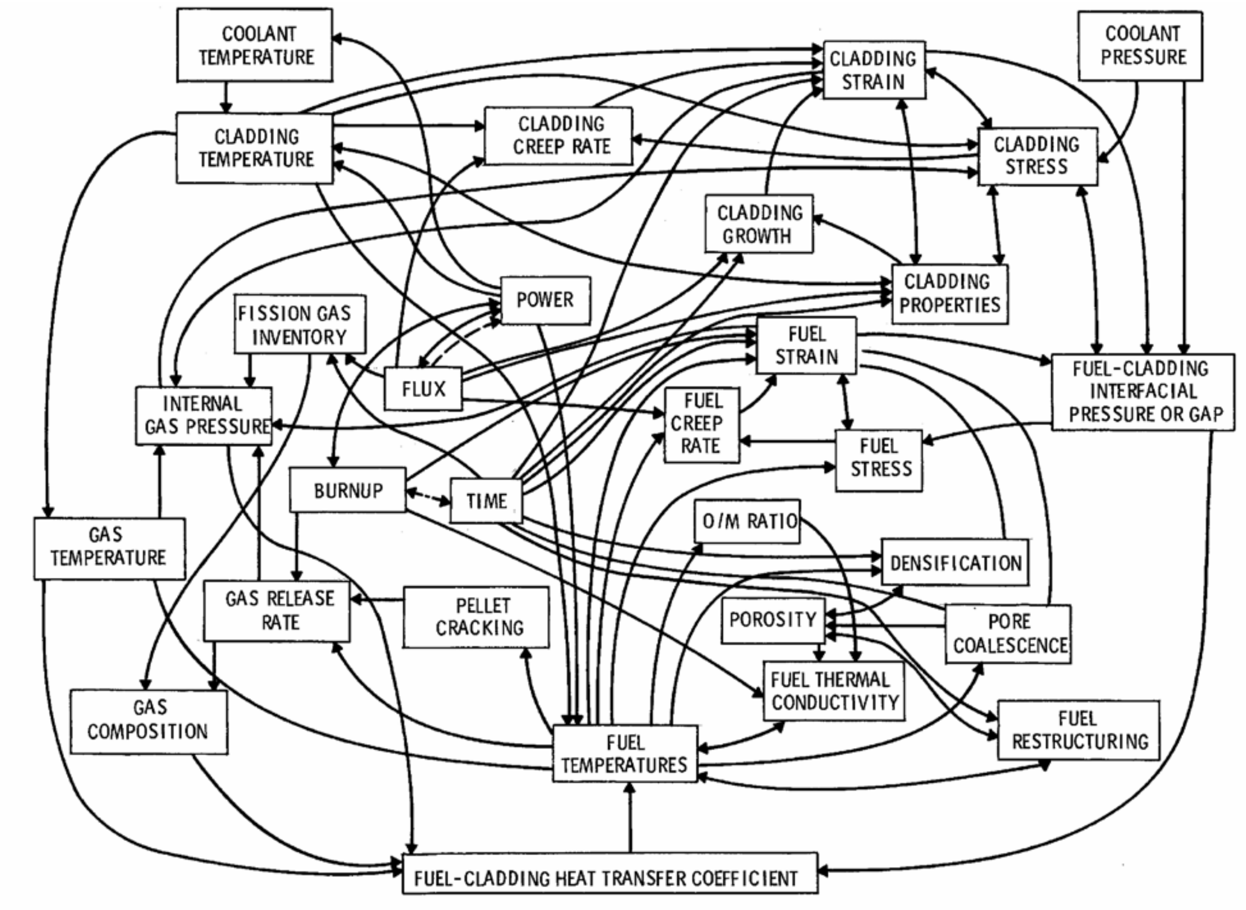
- To interpret full scale experiment results

The CABRI facility (CEA) is a pool-type research reactor dedicated to studying Reactivity Initiated Accidents (RIA) upon a section of Highly-Irradiated fuel. This facility is used to reproduce representative conditions of such accidents.



But…

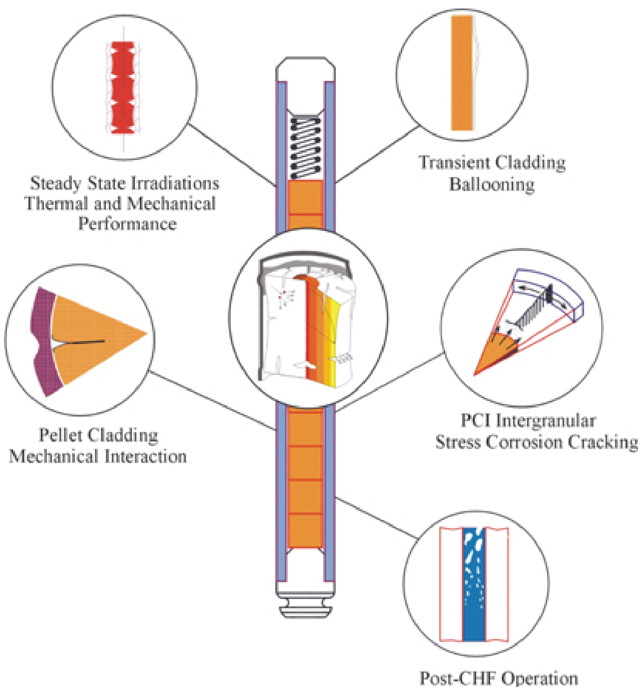
Fuel rod modeling tools for safety analysis

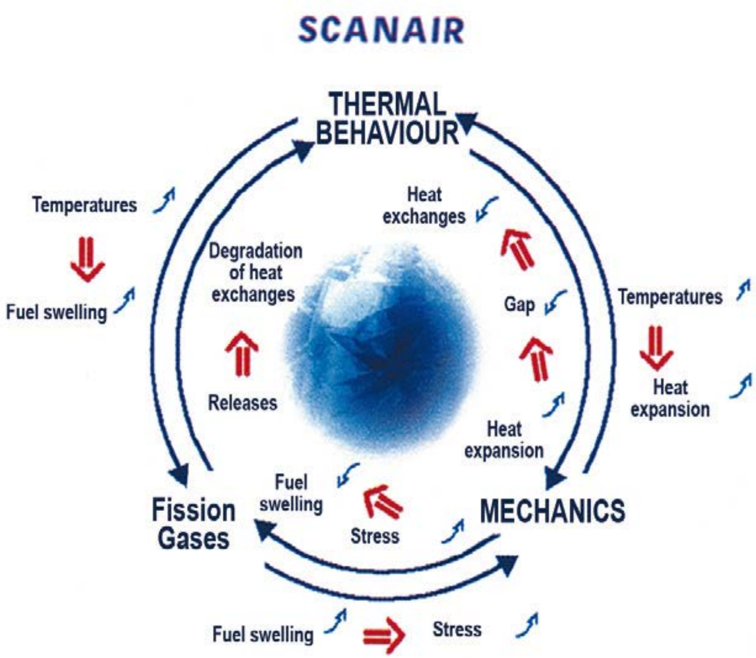


➔ Needs for multi-physics fuel performance code !!

Fuel rod modeling tools for safety analysis

FALCON





Multiphysics code

- Thermal models
- Mechanical models
- Microstructure evolution (cladding oxydation, Fission gaz…)

Fuel rod modeling tools for safety analysis

- Limitation
  - Validity domain : the one used to fit correlations
    - New materials
    - New situations
  - No simple experimental result extrapolation to reactor case

→Need for physical models instead of correlation

Fuel rod modeling tools for safety analysis

- Methodology
  - Elementary mechanisms determination
  - Physical models development
  - Validation on analytical experiment

Yes No

  - Integration of these models into macroscopical simulation tool
  - Validation on full scale experiment and reactor case

Yes No

Reactor case transposition

Fuel rod modeling tools for safety analysis

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relevant time and space scale

  - Integration of these models into macroscopical simulation tool
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Reactor case transposition

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Intragranular fission gas bubble study :

Origin of the gas

Nuclear fission of uranium

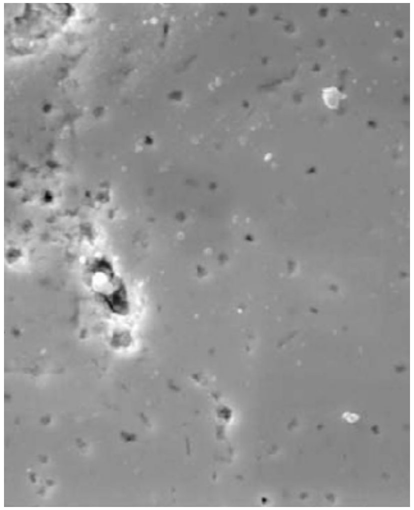
$$^{235}_{92}U + ^{1}_{0}n \rightarrow ^{236}_{92}U \rightarrow X + Y + k\,^{1}_{0}n$$

Gas products (Xe, Kr)

insoluble in the UO_2 matrix

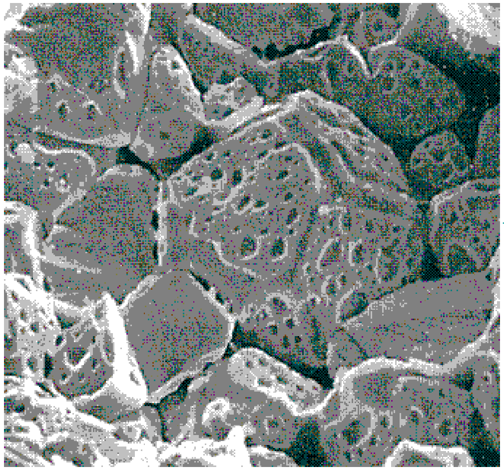
Diffusion to the grain boundaries

Precipitation



Intragranular bubbles (1–10 nm)

T > 1800K

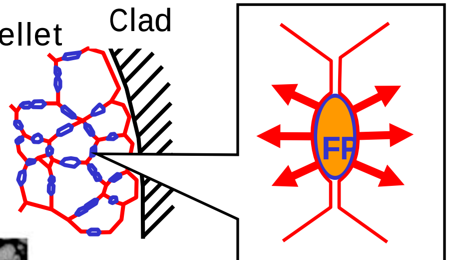


Intergranular bubbles (20–100 nm)

Networks of interconnected bubbles

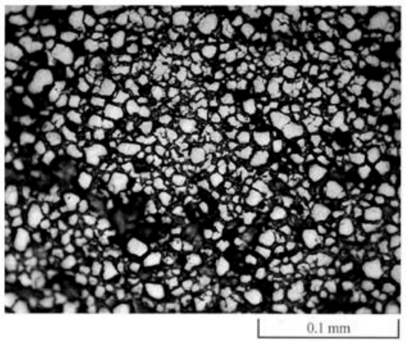
Release in the rod free volume

Intragranular fission gas bubble study :
Ria behavior



at an RIA

TK1 test



Fuel grain boundary decohesion after test

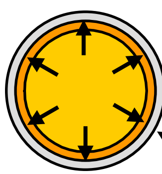
RIA

Prompt increase of fuel temperature

Rapid expansion of accumulated fission gas
Fuel grain boundary decohesion

? Prompt gas release

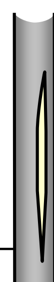
? Gas-induced pellet expansion in early stage of transient



Gas pressure

Enhanced PCMI

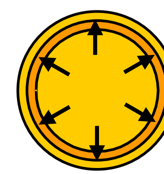
Cold cladding



Gas effect on cladding failure in early stage

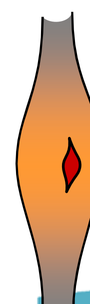
? Delayed gas release

? Post-DNB increase of rod internal pressure



Gas pressure

Hot cladding



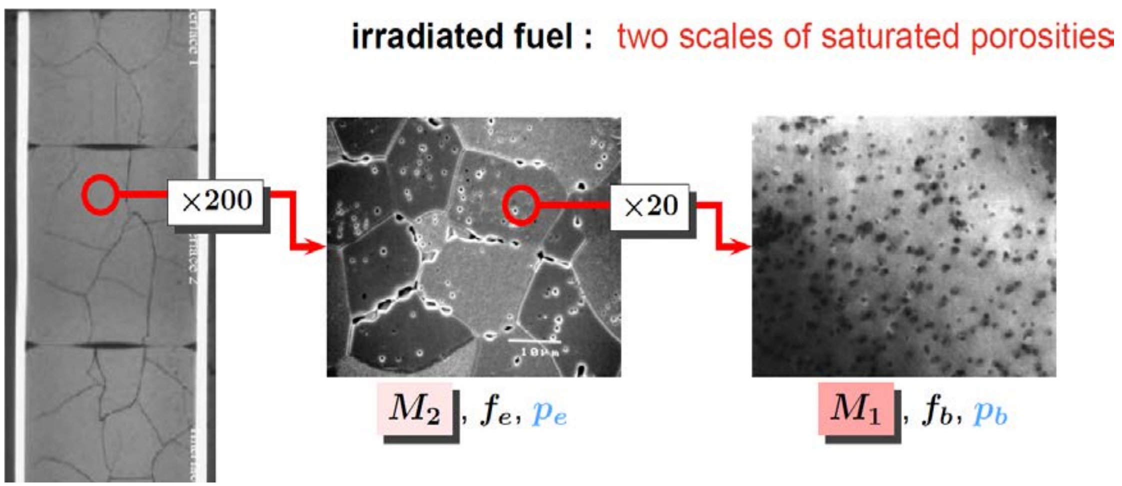
Gas effect on post-DNB failure

➔Knowledge of fission gas behavior = Safety requirement

Intragranular fission gas bubble study :
Pending questions

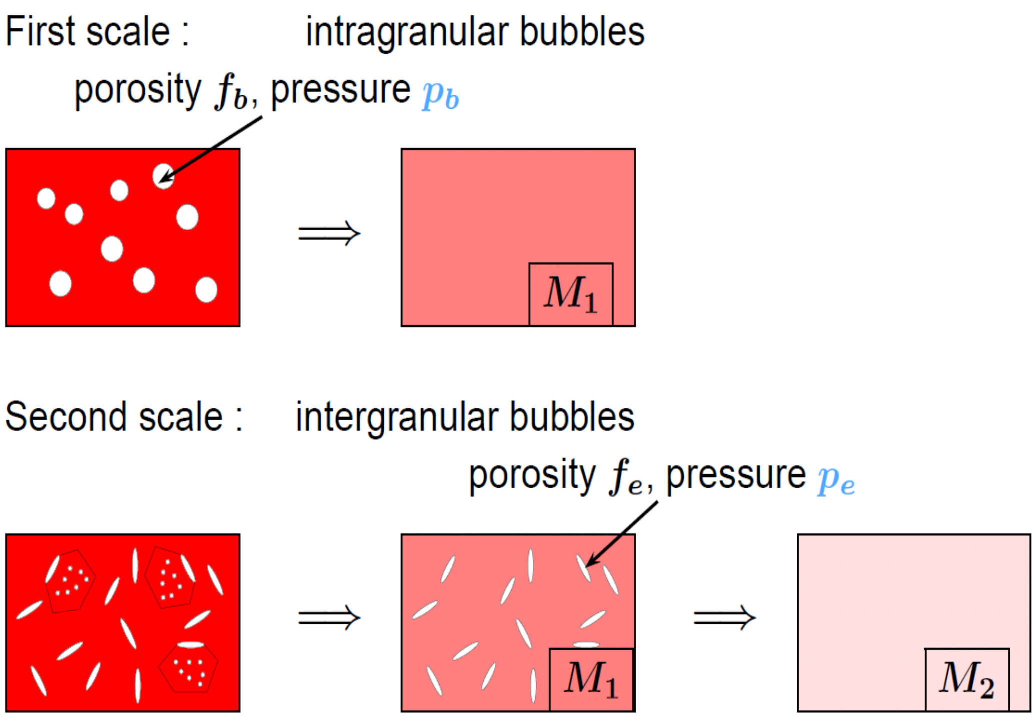
- How the microstructure modifies material properties ?
  - Thermomechanical behavior laws modification
- What is the microstructure time evolution

➔Relevant scale : mesoscopic one



Intragranular fission gas bubble study :
Mesoscopic scale

- Homogenisation approach



Homogeneous equivalent material M_2 with simple thermomechanical behavior law, depending on : matrix properties, porosity shape and value, bubble pressure

Vincent et al., International Journal of Solids and Structures, Volume 46, Issues 3–4, February 2009, Pages 480-506

Intragranular fission gas bubble study :
Mesoscopic scale

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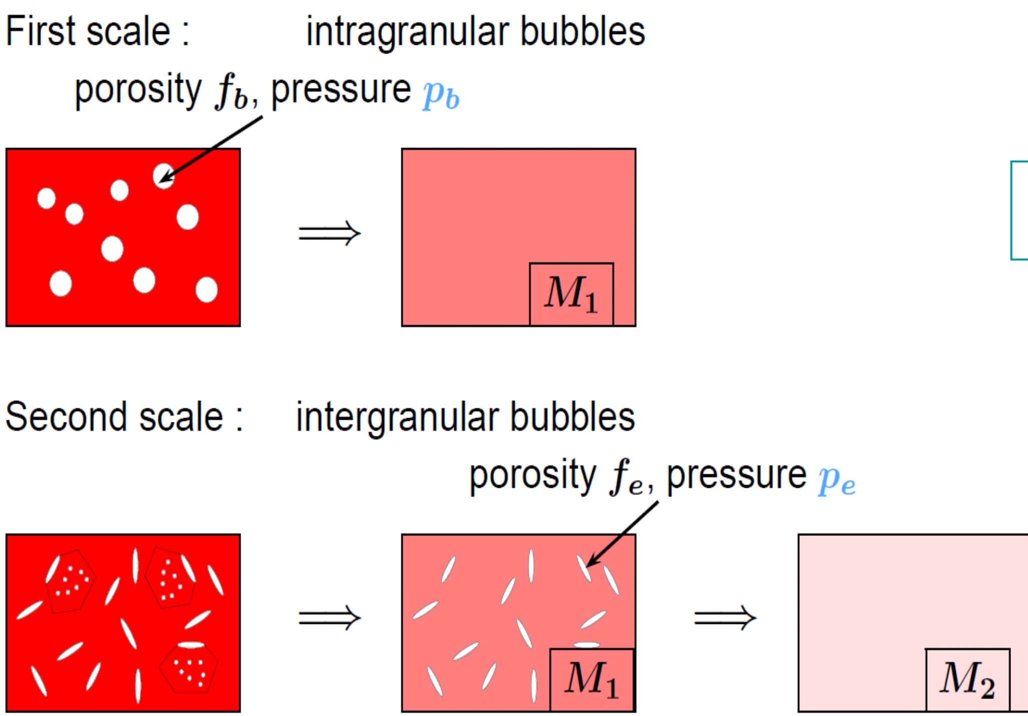

f and p time evolution ?

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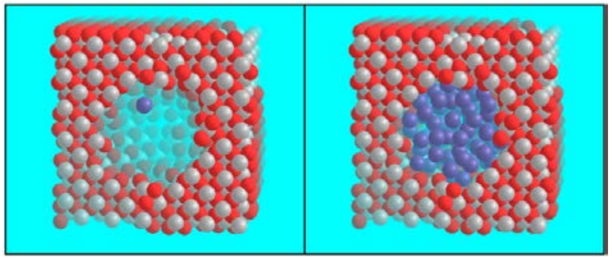
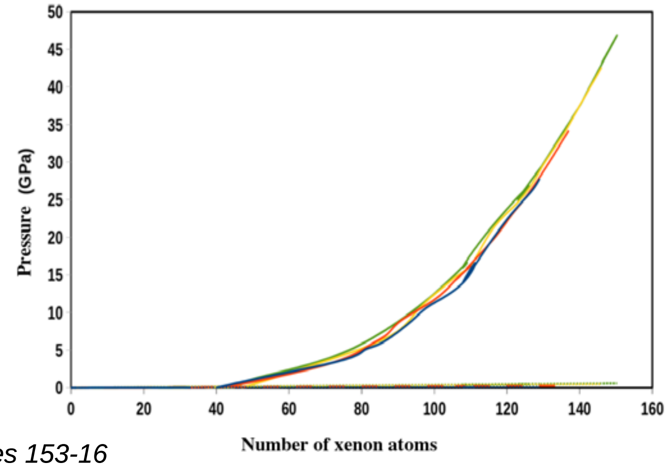
Intragranular fission gas bubble study :
Microscopic scale

- Atomistic study
  - Classical Molecular Dynamics
  - Monte Carlo Approach
  - Analytical model derivation



- Main results
  - Impact on mechanical properties
    - Good agreement with micromechanical and experimental results
    - Surface effects must be taken into account
  - Thermal conductivity :
    - Getting new model → analytic formula
    - Impact of porosity distribution
  - Pressure calculation :
    - Major confinement effect
    - Ideal gas law inadequate/new law to implement

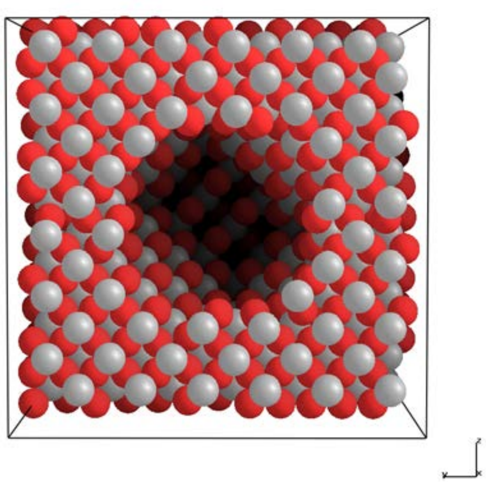


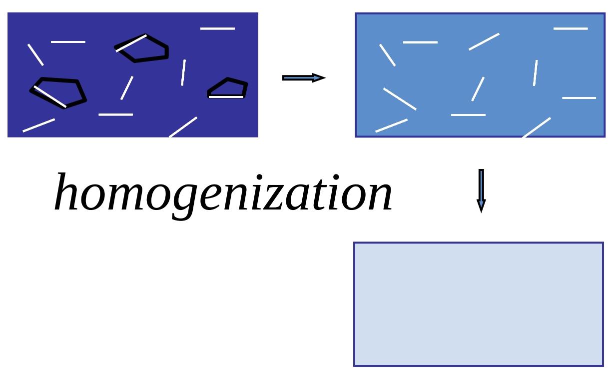
Jelea et al., Journal of Nuclear Materials, Volume 444, Issues 1–3, January 2014, Pages 153-16
Jelea et al., Journal of Nuclear Materials, Volume 415, Issue 2, 15 August 2011, Pages 210-216

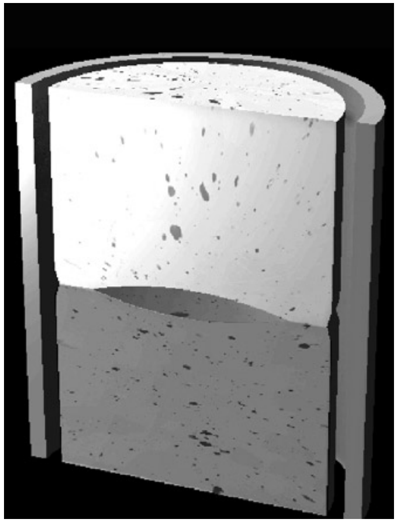
Intragranular fission gas bubble study :
Balance

Bottom-up approach

Atomistic study | *Mesoscopic study* | *Global model*







- $\cancel{P_m = P_g - 2\gamma/R}$
- $\cancel{P_g = NRT/V}$

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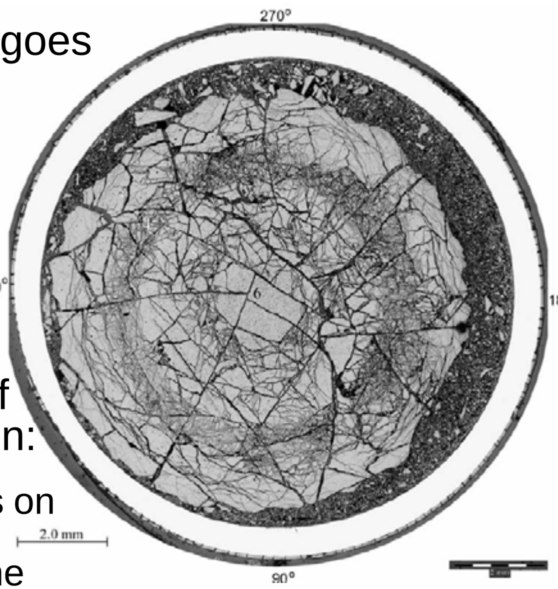
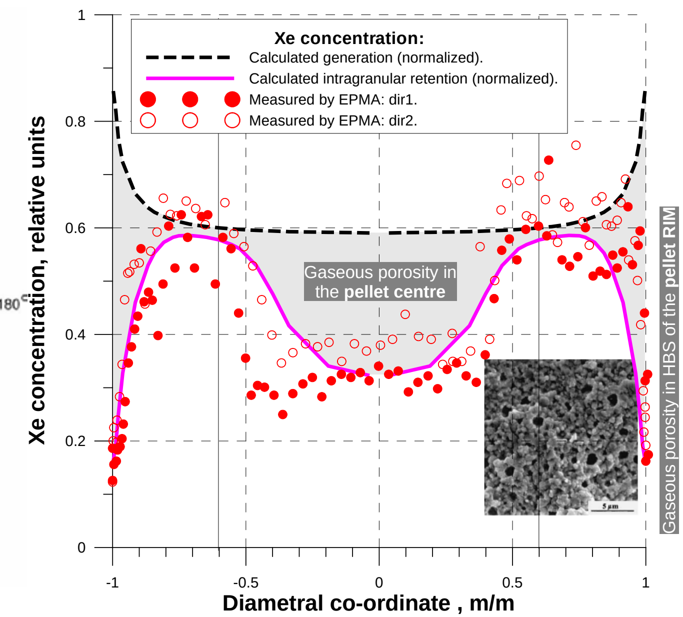
Integral analysis of HBU fuel behaviour in LOCA :

Burst release of the retained fission gas during fuel fragmentation

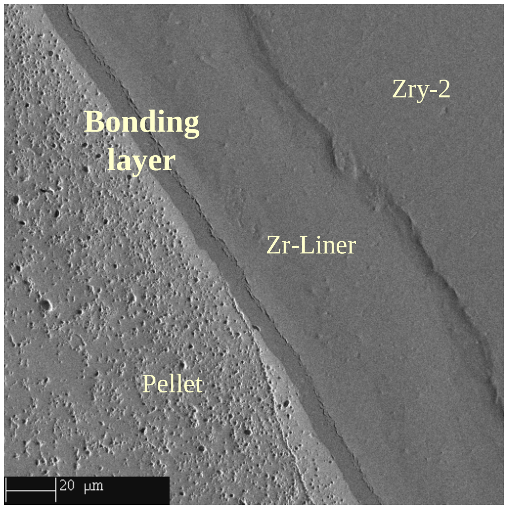
- During LOCA, HBU fuel undergoes significant fragmentation and relocation, which can affect:
  - PCT (‘hot-spot’ effect);
  - Coolability (f. dispersal) …





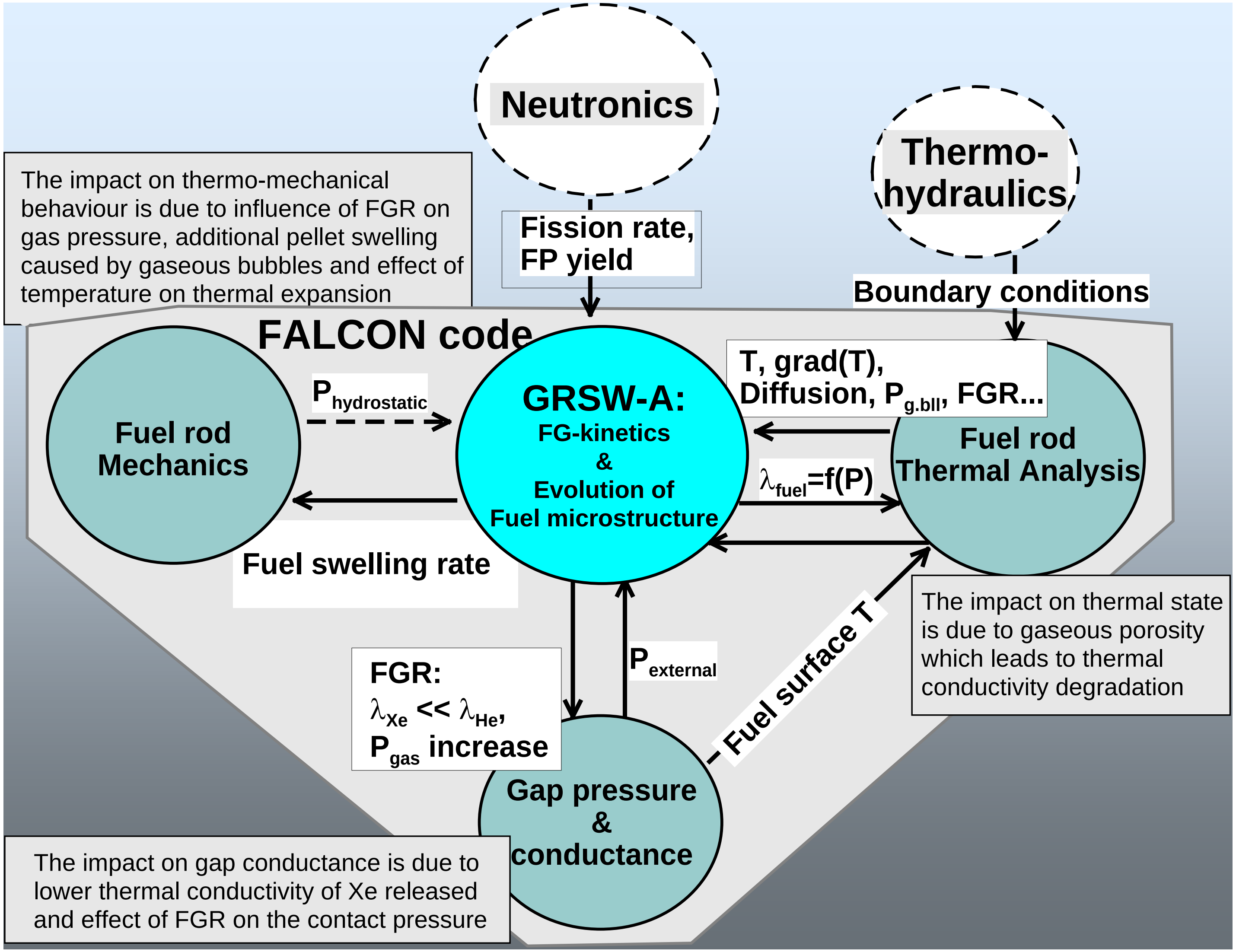
- Fuel micro-structure is to be analyzed from the viewpoint of its effects on fuel fragmentation:
  - Susceptibility to this depends on structural state (e.g. fuel pulverization of the HBS in the rim).

- Also, initial distribution of the retained gas should be analyzed to estimate the quantity and consequences of burst FGR during LOCA



- Considerable quantity of FG can be retained by HBU, and then released during LOCA:
  - FG in gaseous pores in pellet centre, and in HBS pores of pellet rim;
  - Gas can be locked by the pellet-cladding bonding, not reaching the pleanum in the full-scale rod.

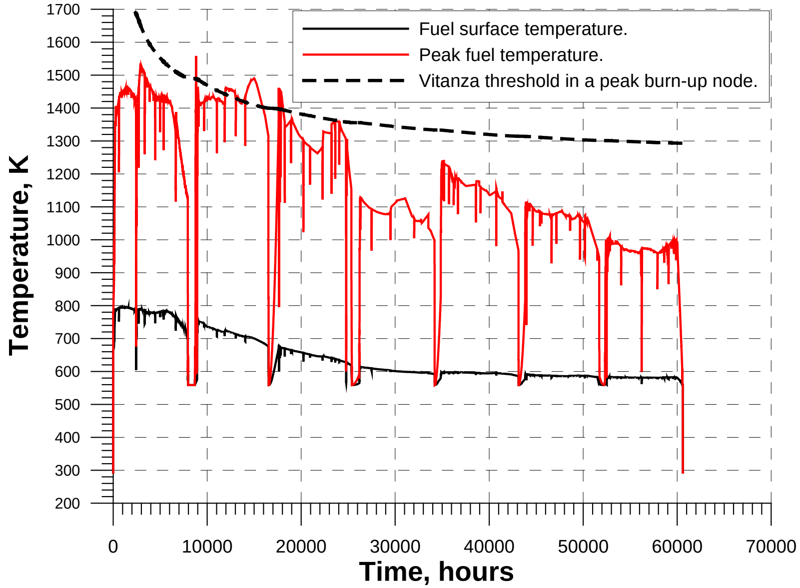
Integral analysis of HBU fuel behaviour in LOCA :
Integration of a mesoscopic model into FALCON FPC analysis

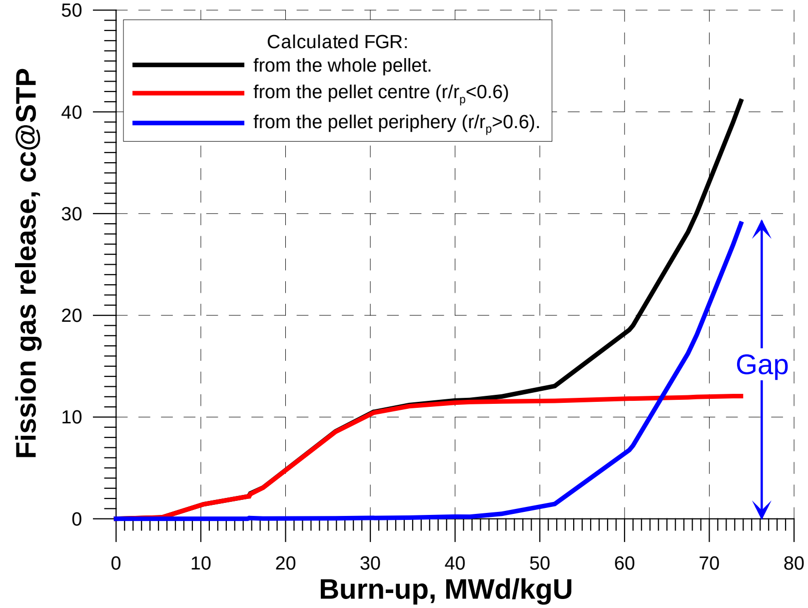


G. Khvostov, K. Mikityuk, M.A. Zimmermann, NED, Vol. 241, Issue 8, August 2011, pp. 2983-3007 (2011)

Integral analysis of HBU fuel behaviour in LOCA :

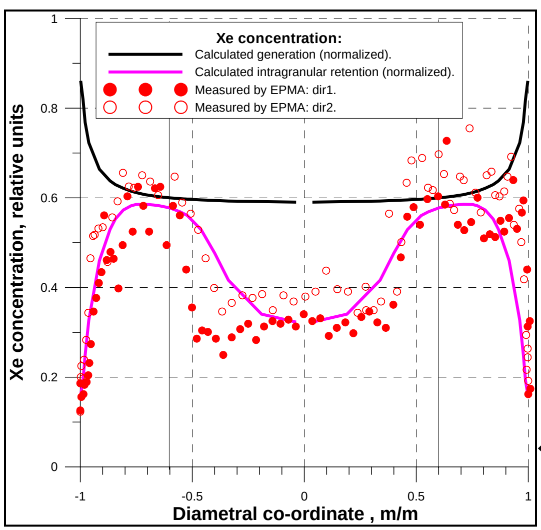
Application of advanced FALCON to estimation of burst FGR





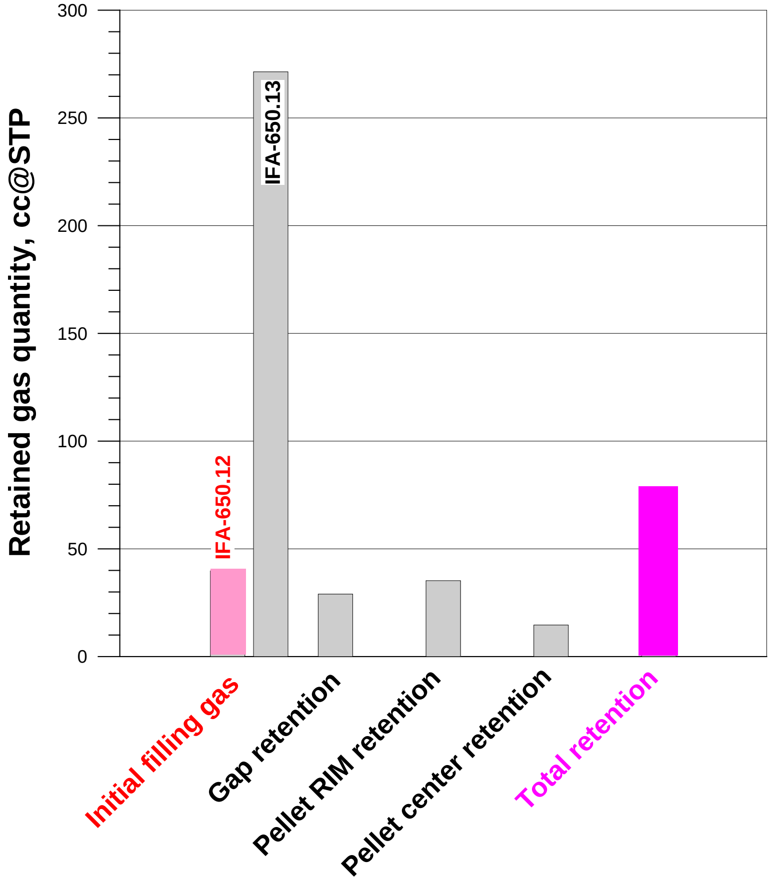
Calculated fuel temperature (left) and decomposition for absolute FGR in segment C of the mother rod (right)

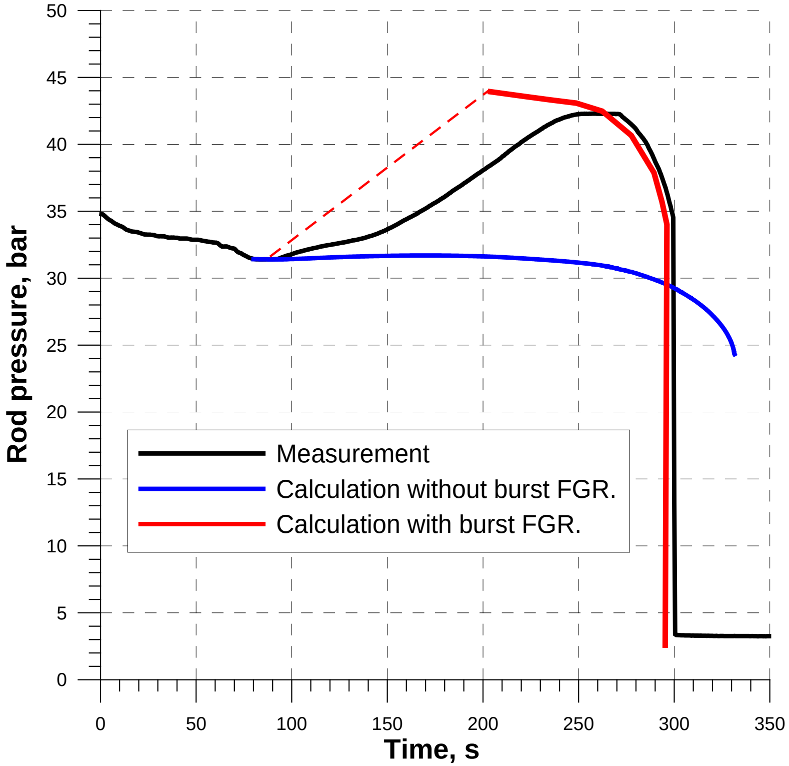
- According to calculation, FGR during the base irradiation was due to: (1) thermally induced release from the pellet centre at medium BU and (2) HBS – assisted release from the RIM at HBU.



- Having calculated FGR during BI as shown above, we capture the features of matrix concentration of Xe across the pellet as measured by EPMA.

Integral analysis of HBU fuel behaviour in LOCA :
Application of advanced FALCON to estimation of burst FGR





- Therefore, effect of such FGR on fuel behaviour during LOCA, particularly on rod pressure, can be important.
- Analysis of such macroscopic transient effects requires meso- and macroscopic consideration of base irradiation
- The quantity of the retained FG, available for transient FGR, is comparable to the initial filler-gas quantity in the rod.

G. Khvostov, et al., "Analysis of Halden LOCA test with the BWR high burnup fuel", 2013 LWR Fuel Performance Meeting / Top Fuel, Charlotte, NC, USA, September 2013, paper 8297.

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Conclusion

- Multi-scale approaches can help to improve safety study
  - Illustration in nuclear fuel rod behavior modelling
    - Identification of predominant physical mechanisms
    - Model parameter determination
  - Needs for experimental validation at each relevant scale
- Similar methodology can be applied to other components
  - Vessel steel for example

Irradiation damages ↔ Microstructure ↔ Macroscopical properties