Reflections on 25 years of LWR fuel modeling, challenges and contemporary issues

A Presentation To The

Nuclear Science and Technology Interaction Program (NSTIP)
Oak Ridge National Laboratory

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LWR Fuel Modeling & Simulation

- Background
- Fuel Modeling & Simulation
- Challenges
  - Fuel-Cladding Gap (Relocation)
  - PCI
  - Fission Gas Release
- Contemporary Issues
- Conclusions

Characteristics of BWR/PWR Fuel and Operation during 1970s

Parameter	PWR	BWR
Residence time	3 yrs	4 yrs
Hot Channel Factor Steady-state Transient	 1.5-2.1 2.3-2.5	 1.8-2.2 2.3-2.5
Neutron Flux Thermal (n/cm^2-s) Fast (n/cm^2-s)	 $4 – 6 \times 10^{13}$ $6 – 9 \times 10^{13}$	 $3 – 5 \times 10^{13}$ $4 – 6 \times 10^{13}$
Burnup target (GWd/tU)	28 - 34	22-28
Fuel Types (No. Plants)	14 x 14 (24) 15 x 15 (28) 16 x 16 (2) 17 x 17 (6)	6 x 6 (7) 7 x 7 (30) 8 x 8 (3) (Intro. 1973) 8 x 8-1 (2) 8 x 8-2 (4)

F. Garzarolli, R. von Jan, H. Stehle, The Main Causes of Fuel Element Failure in Water-Cooled Power Reactors, Atomic Energy Review, **17**, 1 (1979)

Historical BWR Ramp Programs

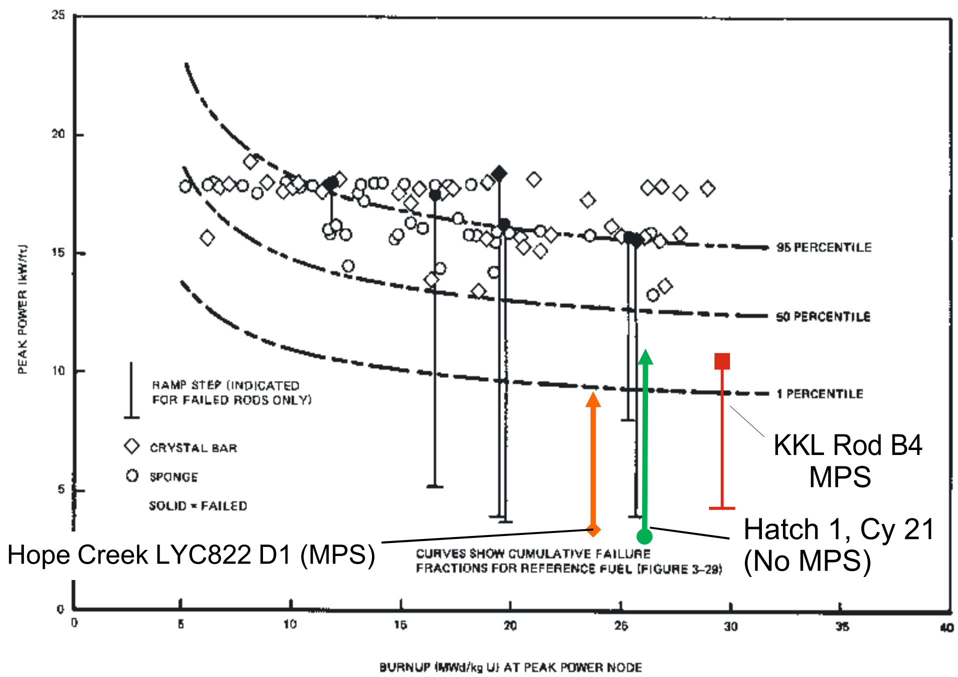
- Inter-Ramp (1977-1978)
  - Twenty 8x8 Fuel Rods
    - » 11 failures
- Demo-Ramp
  - Demo-Ramp I (Dec 1981): Five 8x8 Fuel Rods
    - » no failures
  - Demo-Ramp II (2Q80 – 1Q81): Nine 8x8 Fuel Rods
    - » 1 failure, 5 incipient failures
- Super-Ramp I (1980-1983)
  - Eight KWU 8x8 Fuel Rods
    - » 3 failures
  - Eight GE 8x8 Fuel Rods
    - » 4 failures
- Trans-Ramp I (1982-1984)
  - Five KWU 8x8 Fuel Rods
    - » 2 failures

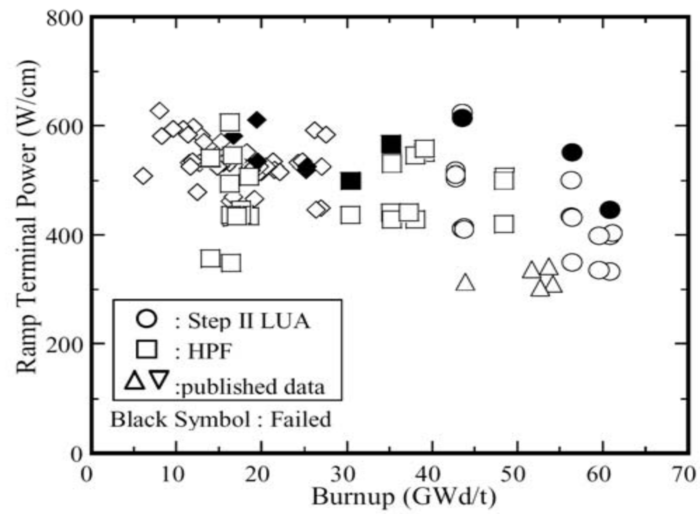
BWR Ramp Tests – GE (GNF) / Toshiba

Hiroshi Sakurai et al "Irradiation Characteristics of High Burnup BWR Fuels", Proceedings of the ANS 2000 International Topical Meeting on LWR Fuel Performance, Park City, April 2000.

Hiroshi Hayashi et al, "Outside-in Failure of High Burnup BWR Segment Rods Caused by Power Ramp Tests," TOPFUEL 2003.

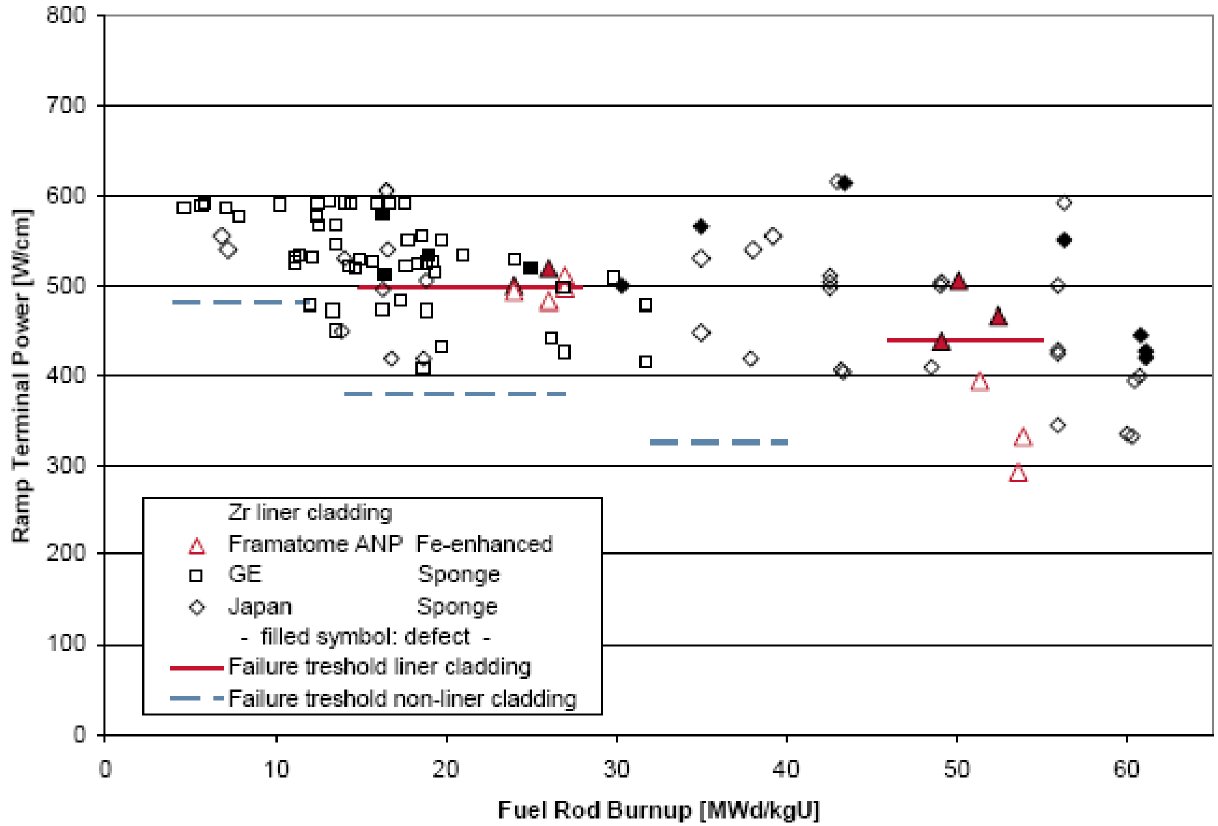
Barrier ramp test results (open = sound, solid = failed)
Curves show cumulative failure fractions
for reference, i.e. non-barrier fuel





MPS = Missing pellet surface

Results of Siemens Ramp Test on Fe-Enhanced Liner Cladding

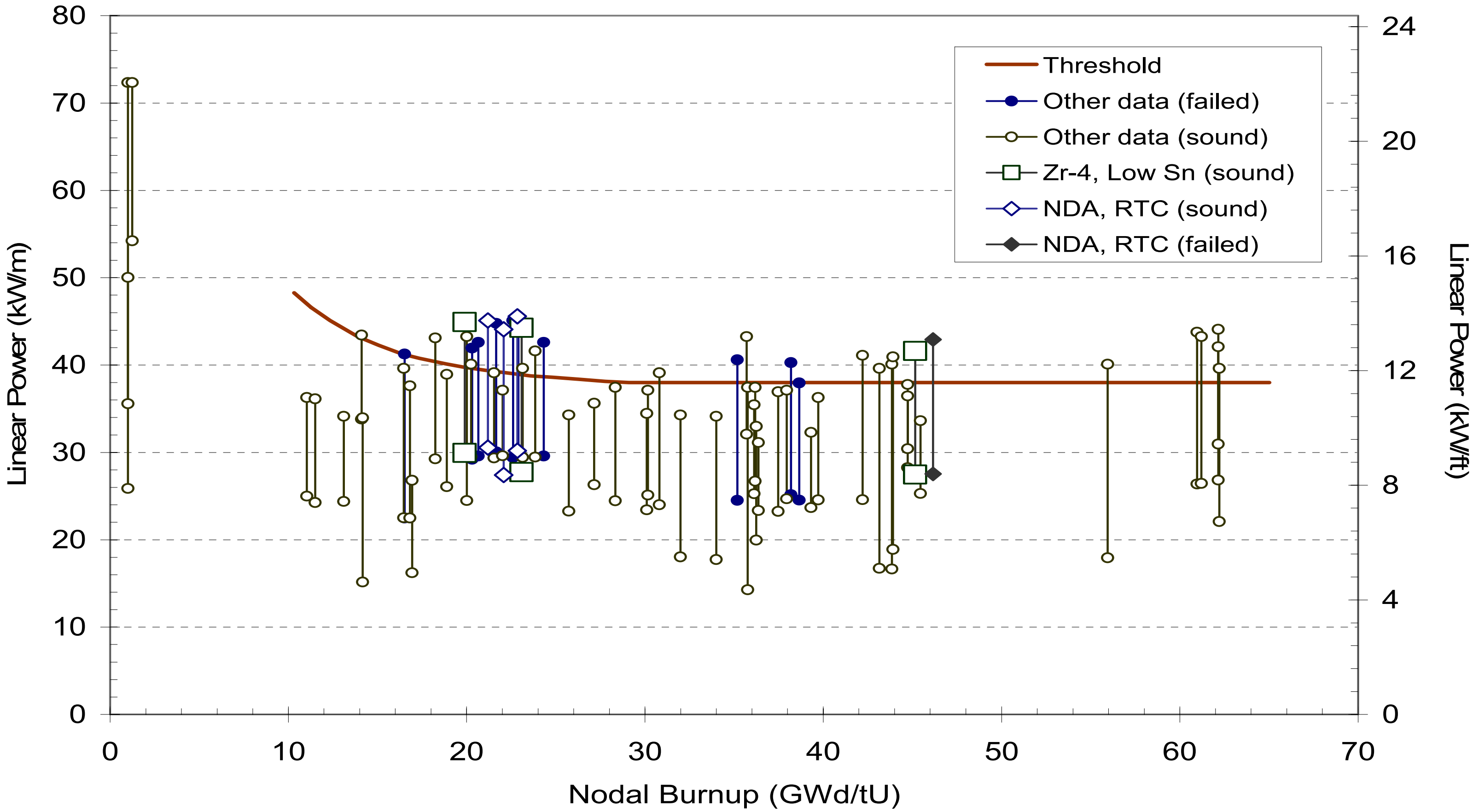


P. B. Hoffmann, P. Dewes, "Post-Irradiation Examination and Ramp Testing of Fuel Rods with Fe-Enhanced Linear Cladding at High Burnup, Proceedings of the 2004 International Meeting on LWR Fuel Performance, Orlando, 2004, pp. 238-243.

Historical PWR Ramp Programs

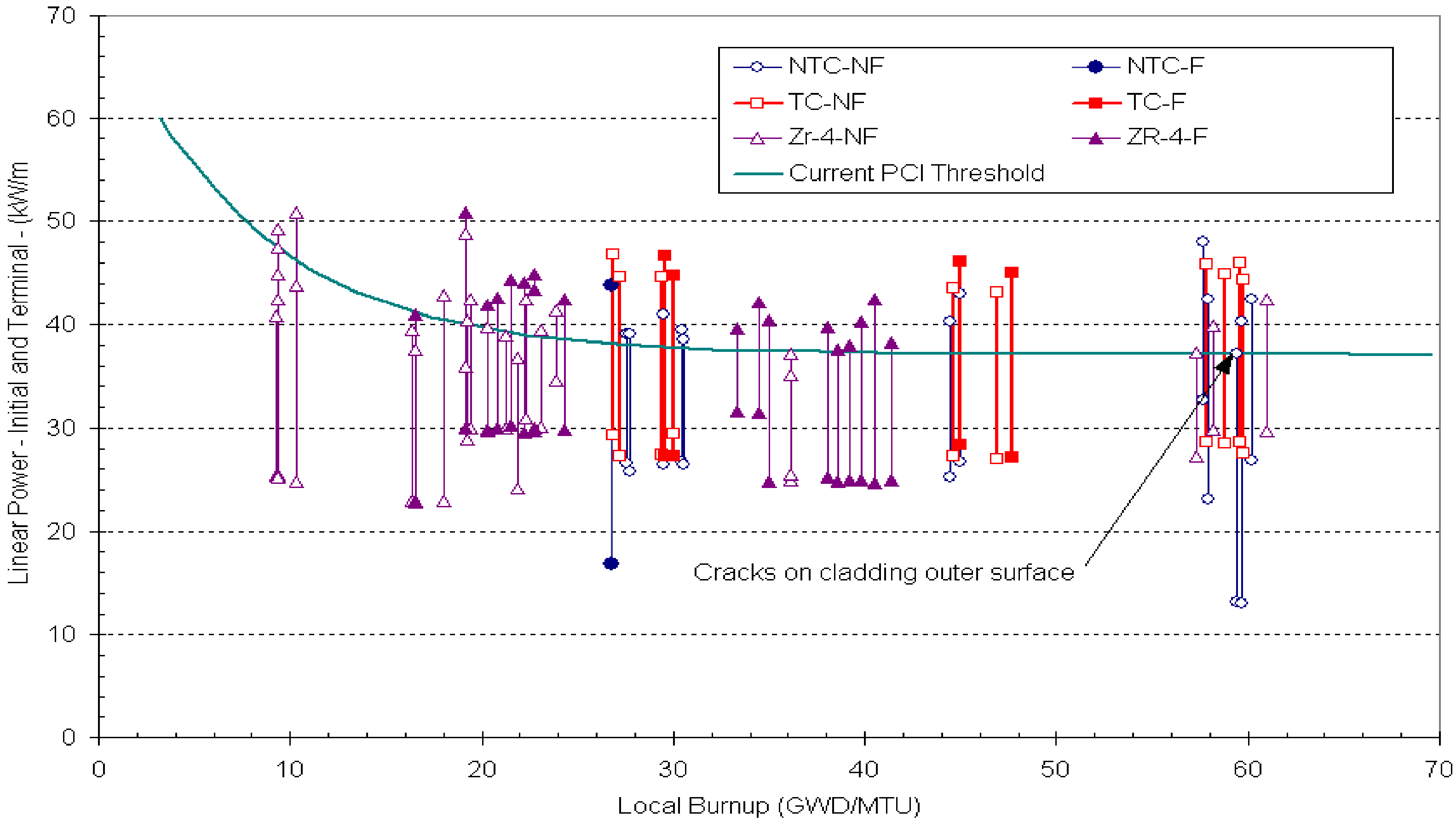
- Over-Ramp
  - (1978 -1979): 5 W (17x17) Fuel Rods
    - » 7 failure
  - (1977 -1979): 24 KWU/CE (14x14) Fuel Rods
    - » 7 failures
- Super-Ramp I (PWR)
  - (1980-1981): 19 KWU (14x14) Fuel Rods
    - » 2 failures
  - (1981-1982): 9 W (17x17) Fuel Rods
    - » 7 failures
- Trans-Ramp II
  - (1984 -1986): 6 W (17x17) fuel rods
    - » 3 failures
- Trans-Ramp IV
  - (1989 -1993): 7 Fragema (17x17) Fuel Rods
    - » 2 failures

NFI Ramp Test Program (NDA and Zr-4)



K. Goto et al, "UPDATE ON THE DEVELOPMENT OF JAPANESE ADVANCED PWR," Proceedings of the ANS 2000 International Topical Meeting on LWR Fuel Performance, Park City, April 2000.

Mitsubishi Ramp Test (MDA and Zr-4)



Yoshiaki TSUKUDA(NUPEC), Yuji KOSAKA, Toshiya KIDO(NDC), Soichi DOI(MNI), Toshikazu SENDO(KEPCO), Pedro GONZÁLEZ(ENDESA), J.M.ALONSO(ENUSA), “Performance of Advanced Fuel Materials for High Burnup,” TOPFUEL 2003.

Evolution in Fuel Designs and Operations

- 1980s
  - PWR: 17x17 plants (3 loops, 157 assy; 4 loops, 193 assy) become the standard
  - BWR: 9x9 fuel introduced by Siemens & Exxon (ANF) and SVEA-64, SVEA-100 designs introduced by ABB
  - 3 annual cycles for PWR fuel, 4 annual cycles for BWR fuel standard
  - Consideration for higher burnup and 18-month cycles in US initiated
  - Annual cycle length 270-330 efpd
  - Discharge burnups increase to mid-40s GWd/tU
- 1990s
  - 4-5 annual cycles (Europe), shorter lifetime with recycling
  - 3 x 18-mo (18-mo cycle 460-510 EFPD)
  - Consideration for 24-mo cycles, moderate duty PWRs (14x14, 15x15, 16x16) and BWRs
  - GNF/Siemens(AREVA) introduce advanced 9x9 and start development of 10x10 fuel

Evolution in Fuel Designs and Operations (Cont’d)

- 1990s
  - 24-mo cycle (600-690 EFPD)
  - 19-20-21 mo cycle schedule at one PWR plant
  - Discharge burnups increase to 50 GWd/tU
  - Utilities start power uprates: MUR (< 2%), Stretch (< 7%), Extended (<20%).

- 2000s
  - Most 14x14, several 15x15 plants, and some 16x16 plants on 24-mo cycles. Batch sizes approaching ½ core in some cases.
  - Many US BWRs move to 24-month cycles
  - Plant uprates continue
  - High capacity 18-mo cycles approach 530 EFPD

Fuel Modeling Codes

- Vendor codes
  - PAD (Westinghouse)
  - GESTR (GE)
  - FATES (CE)
  - COMETHE (Belgonucleaire)
  - COPERNIC (Framatome, developed from TRANSURANUS)
  - STAV (ABB)
  - TACO (B&W)
- Research organizations and utilities
  - ENIGMA (CEGB/British Energy and BNFL)
  - ESCORE (EPRI), FREY (EPRI) => FALCON (EPRI)
  - TRANSURANUS (ITU, Karlsruhe)
  - INTERPIN (Studsvik)
  - METEOR (CEA, developed from TRANSURANUS)
  - CYRANO (EdF)
  - FRAPCON/FRAPTRAN (PNL / NRC)

Important Fuel Phenomena

- Pellet
  - Pellet thermal conductance (as function of temperature and burnup)
  - Thermal Expansion
  - Densification
  - Swelling (Solid and Gaseous)
  - Cracking
  - Relocation
  - Bonding with Clad
  - Fission Gas Release
  - Fabrication Imperfections (e.g., MPS)
- Cladding
  - Stress Relaxation
  - Creepdown
  - Irradiation Hardening
  - Thermal Expansion
  - Oxidation/corrosion and crud deposition
  - Hydrogen pickup (and hydride precipitation and dissolution)
  - Growth

For both fuel pellets and cladding: Microstructural evolution as functions of exposure and temperature

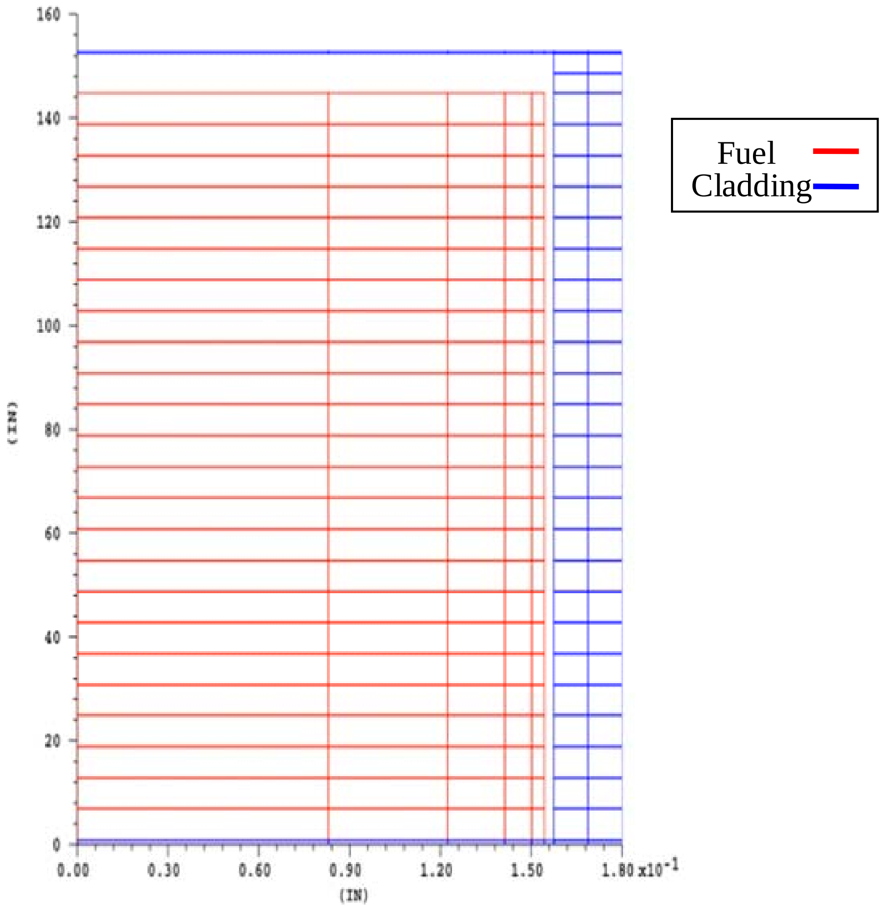
Fuel Modeling Codes (1980s)

- 1-D or 1-1/2 D
  - Axisymmetric, stacked rings/slices of fuel
    - » assume pellets and cladding are concentric/coaxial)
  - Decoupled mechanics (radial and axial decoupled)
    - » e.g., in ENIGMA (1988), coupling between axial zones (slices) restricted to coolant enthalpy/temperature solution, rod internal pressure, and gas transport
    - » "A one-dimensional axi-symmetric mechanical calculation is performed for each axial zone under the assumption of generalised plane strain in both pellet and cladding."

P. A. Jackson, J. A. Turnbull, R.J. White, "A description of the ENIGMA fuel performance code," (IAEA-TC-659/1.2), Water Reactor Fuel Element Computer Modelling in Steady State, Transient and Accident Conditions, Proceedings of A Technical Committee Meeting Organized by the International Atomic Energy Agency, Preston, 18-22 September 1988

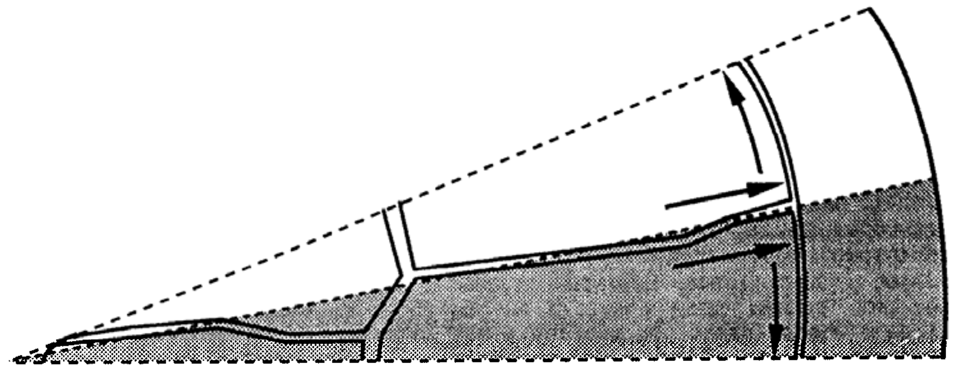
Modeling – FALCON R-Z

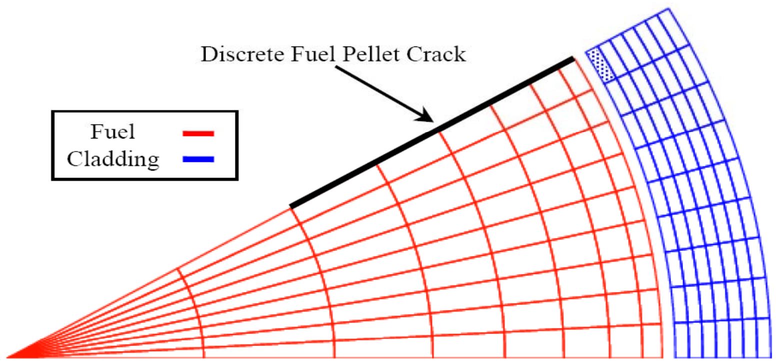
Typical PWR Model

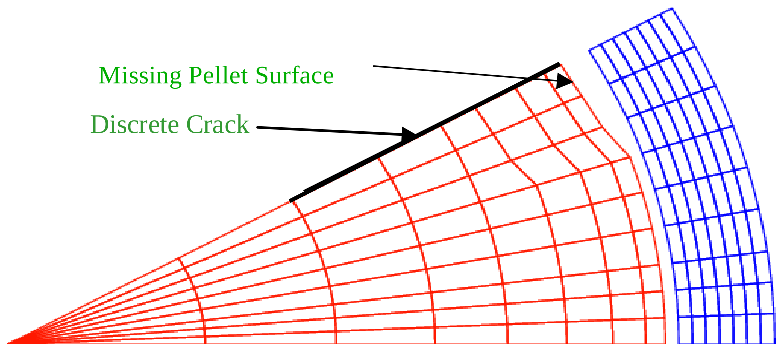


- Elements:
  - 120 Fuel
  - 70 Cladding
    - » 48 active fuel
    - » 4 top plenum
    - » 8 top endplug
    - » 2 bottom plenum
    - » 8 bottom endplug
  - 71 Gap
    - » 49 active fuel
    - » 11 top plenum
    - » 11 bottom plenum
- Nodes:
  - 906 nodes
- Run time: 14 minutes per reactor cycle with coarse time-stepping, with limited fine time stepping at EOC and BOC (Startup)

FALCON R-θ PCI Model (Small)





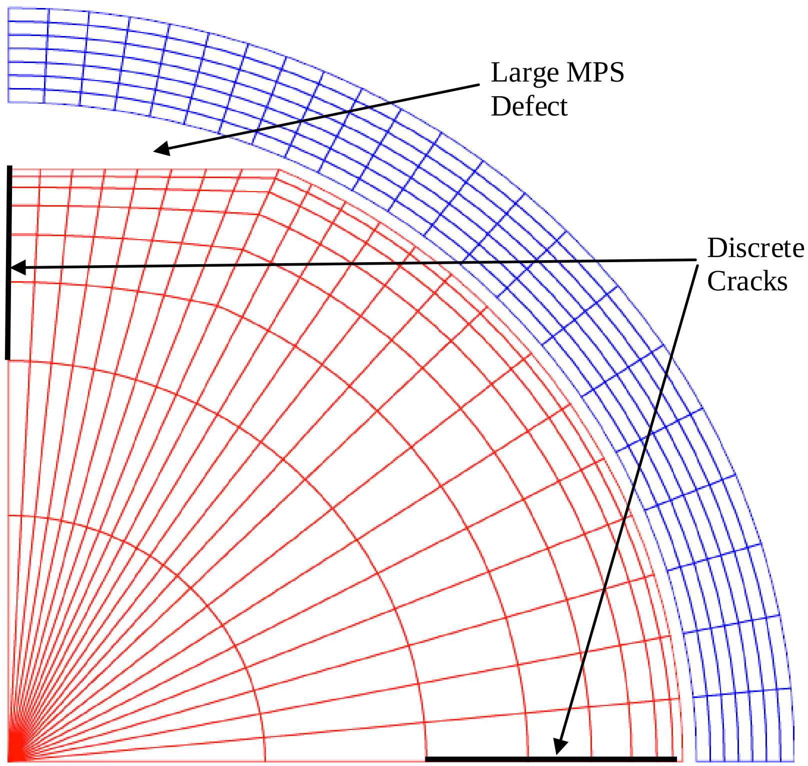


Elements: 72 Fuel + 63 Cladding = 135 total, Gap Elements: 19

Nodes: 251 Fuel + 221 Cladding = 473 total

128 Time steps => Run time ~ 2 min (BOC Startup)

Large MPS R-θ PCI Model (Large)

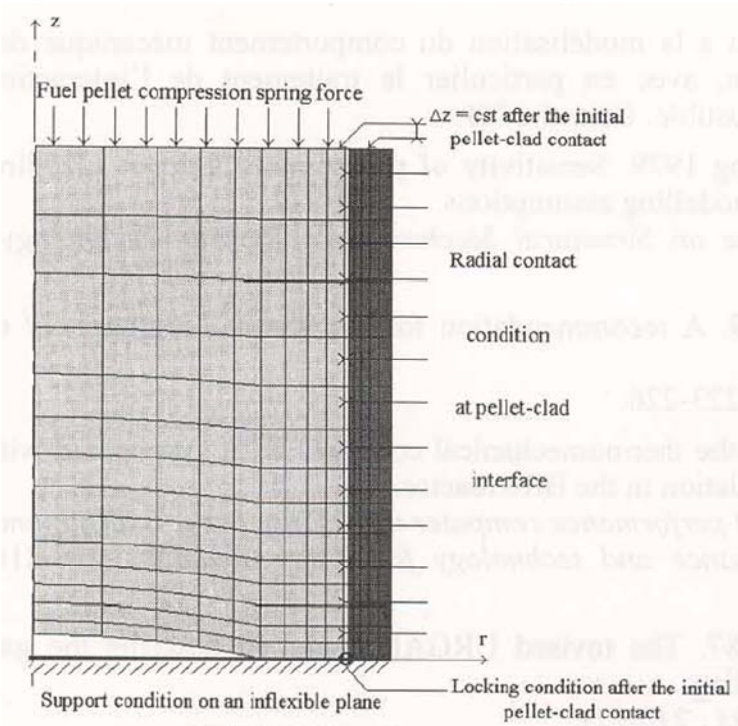


Elements: 176 Fuel + 154 Cladding = 330 total, Gap Elements: 45

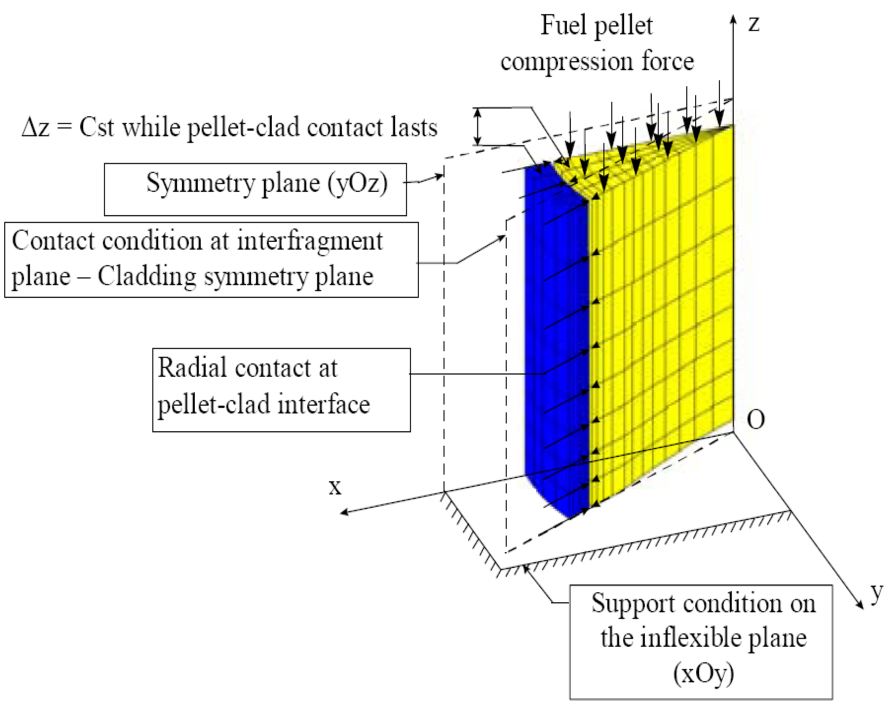
Nodes: 589 Fuel + 521 Cladding = 1110 total

128 Time steps => Run time ~ 10 min (BOC Startup)

Contemporary Simulation Methods - 1

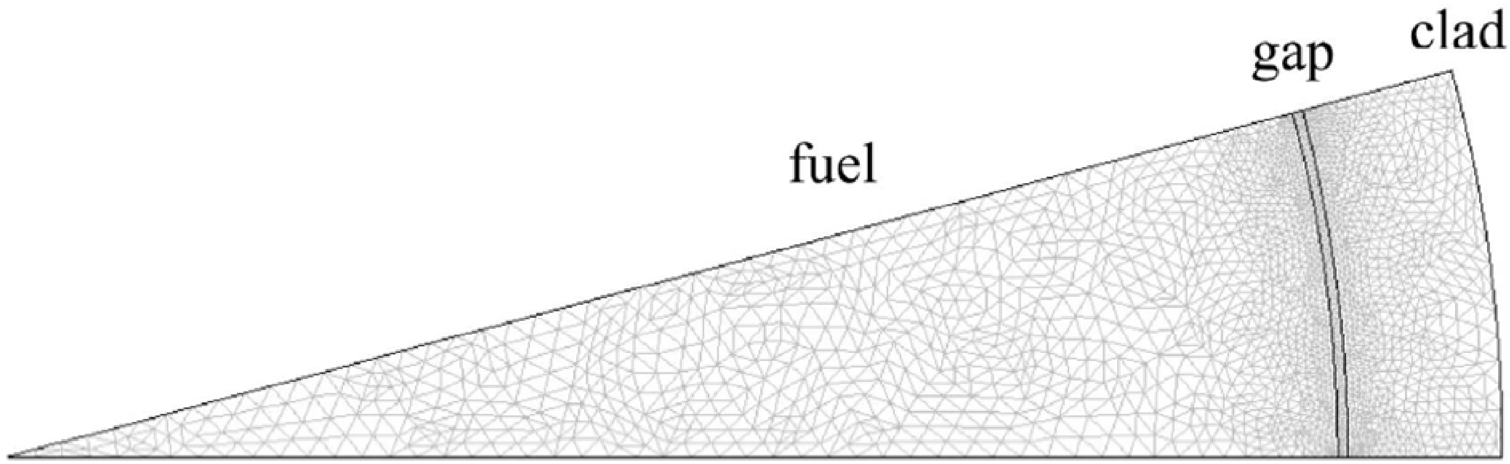


Brochard, J., Bentejac, F., Hourdequin, H., “Nonlinear Finite Element Studies of the Pellet-cladding Mechanical Interaction in a PWR Fuel”, SMIRT 14, France, 17-22 August 1997.



F. Bentejac et al, Fuel Rod Modelling During Transients: The Toutatis Code, "Nuclear fuel behaviour modelling at high burnup and its experimental support," Proceedings of a Technical Committee meeting, Windermere, United Kingdom, 19–23 June 2000

Contemporary Simulation Methods - 2

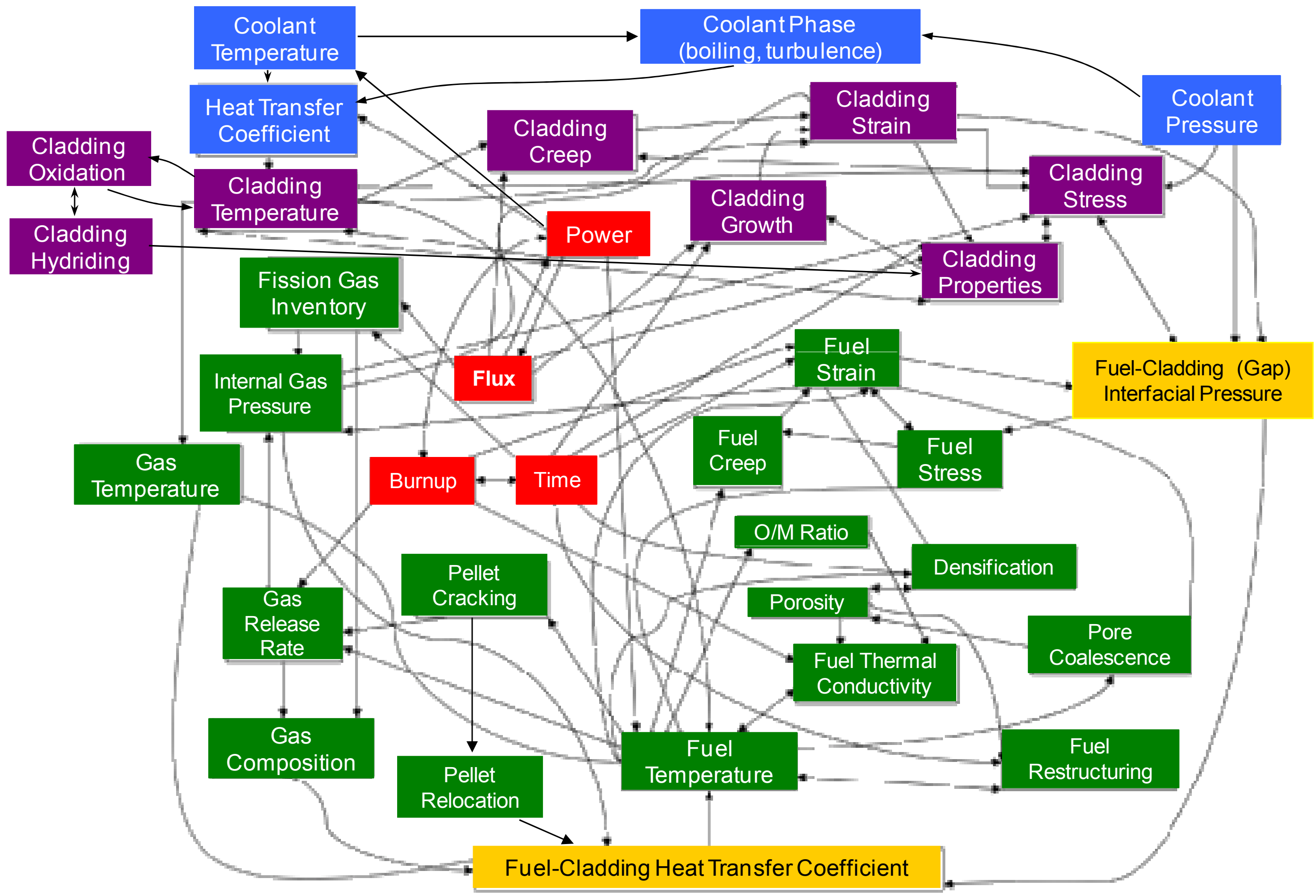


Mesh Refined at fuel-cladding gap, where temperature, stoichiometry and composition gradients are steeper

Mesh elements approaching fuel grain size

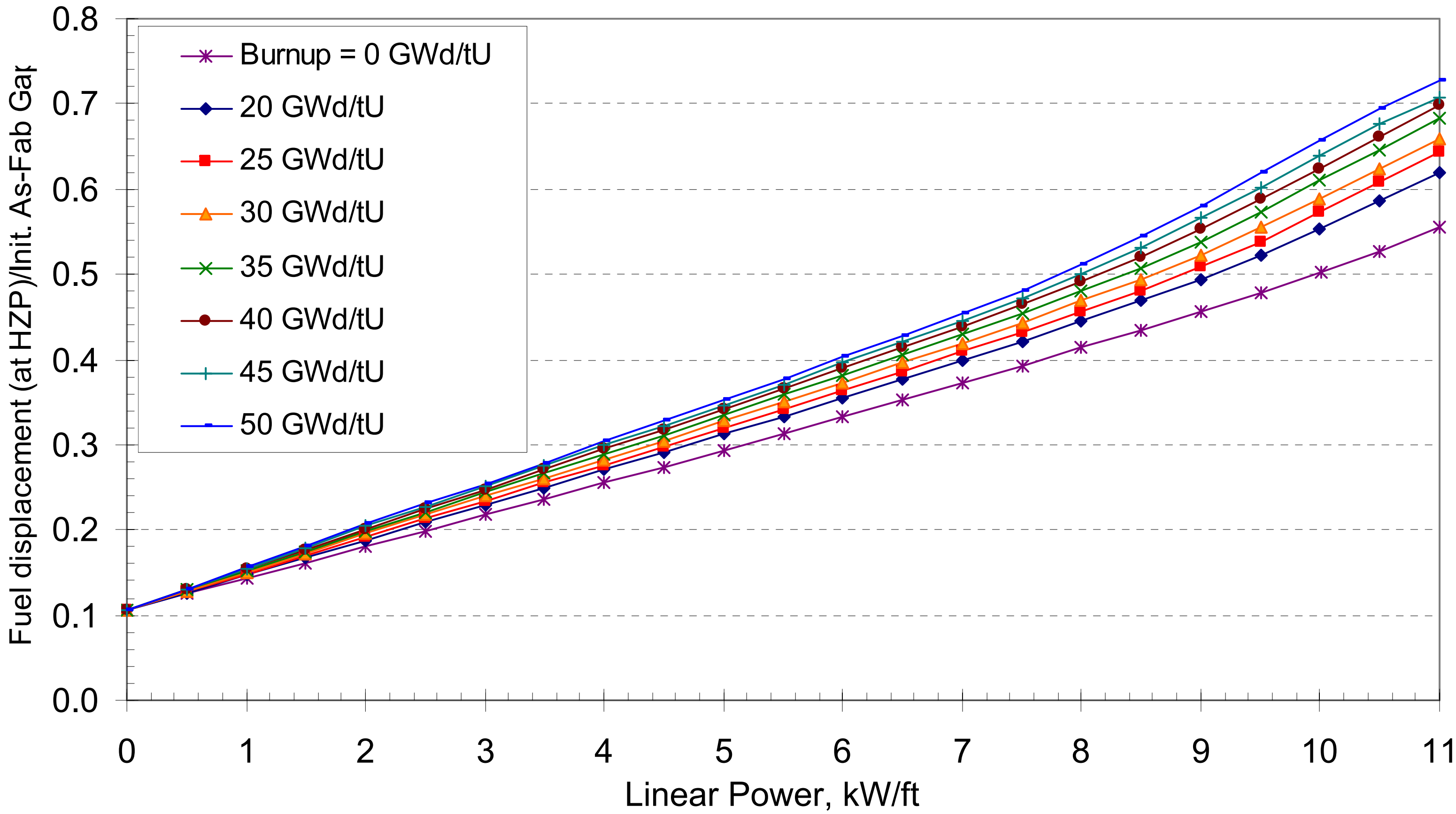
Marius Stan, “Multi-Scale Models and Simulations of Nuclear Fuels,” Nuclear Engineering and Design, Vol.41 No.1 Feb 2009

Complexity of Nuclear Fuel Simulation

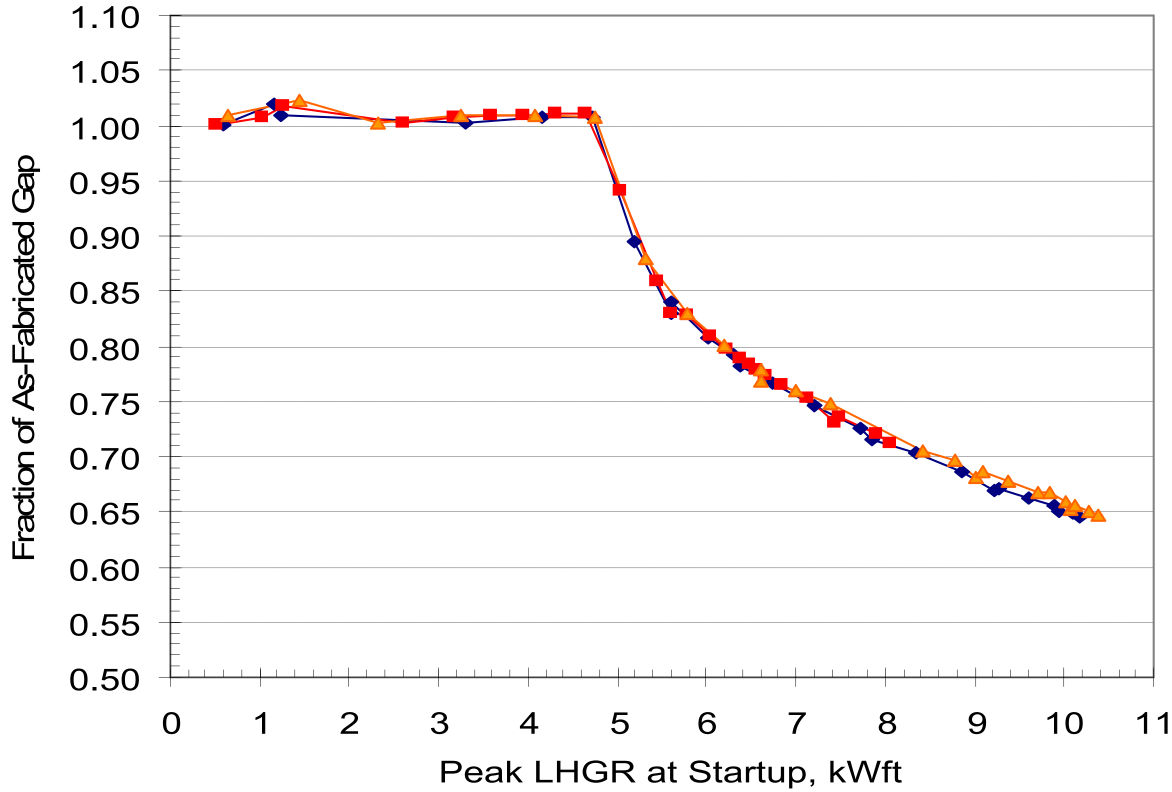


Adapted from K. Lassmann, "The Structure of Fuel Element Codes," Nuclear Engineering and Design, 57 (1980), 17-39.

Fuel Pellet Displacement due to Thermal Expansion as Function of Burnup and Local Linear Power



Impact of Pellet Relocation



Effect of Pellet Relocation on Gap Size as Expressed as Fraction of As-Fabricated Gap Determined by FALCON Analysis of Three BWR Fuel Rods

Relocation Models - 1

FALCON (ESCORE Relocation Model)

$(\%\Delta D/D_o)_{REL} = 0.8\ Q\ (\%G_t/D_o)\ (\ 0.005\ BU^{0.3} - 0.20D_o + 0.3)$

with:

$Q = 0$ for $q' \leq 6$ kW/ft (197 W/cm),

$Q = (q' - 6)^{1/3}$ for 6 kW/ft $< q' \leq 14$ kW/ft (459 W/cm)

where

$(\%\Delta D/D_o)_{REL}$ = percentage change in diameter due to relocation

D_o = as-fabricated cold pellet diameter (inch)

q' = pellet average linear heat rate (kW/ft)

BU = pellet average burnup (MWd/tU)

G_t = the as-fabricated cold diametral gap (inch)

Krammen, M.A., Freeburn, H. R., Eds., *ESCORE-the EPRI Steady-State Core Reload Evaluator Code: General Description*, EPRI NP-5100 (NP-4492 Proprietary), Electric Power Research Institute, Palo Alto, California, February 1987.

Relocation Models - 2

$$R^m(E,q) = H(q-q_c)R_P R^{\infty}\kappa(E)\left[1-e^{-0.154(q-q_c)}\right]$$

$$\kappa(E) = 1 - 0.338e^{-0.15E}$$

where:

R^m = Radial displacement

E = local exposure (MWd/kgU)

q = local linear power density (kW/m)

q_c = 4 kW/m (threshold for relocation)

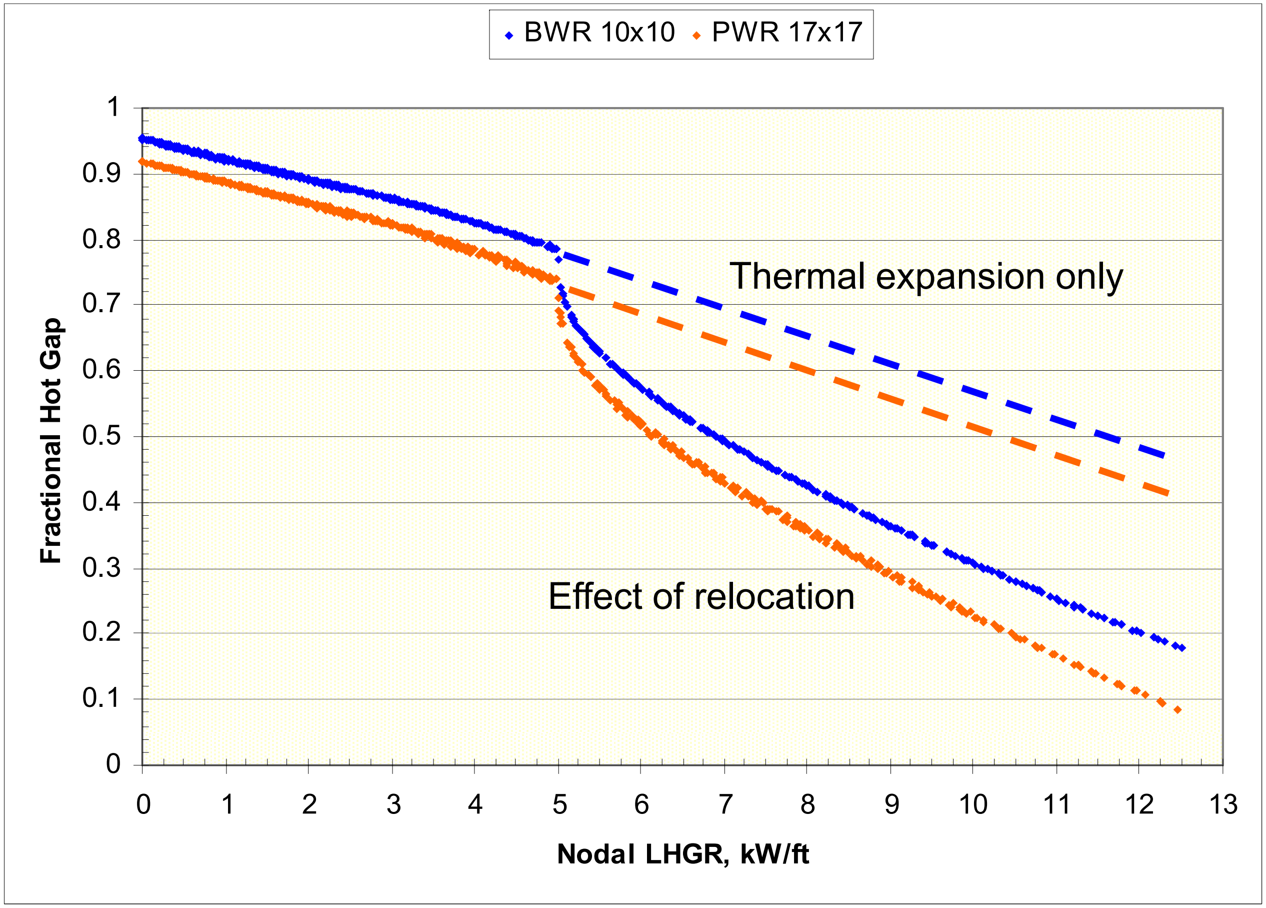
$H(q-q_c)$ = Heaviside function

R^{∞} = calibration parameter (= 0.006 in steady-state, 0.00755 in ramp) deciding the asymptotic limit of pellet relocation

P_n^m = minimum contact pressure to 'fully remove' the relocation (implies recovery)

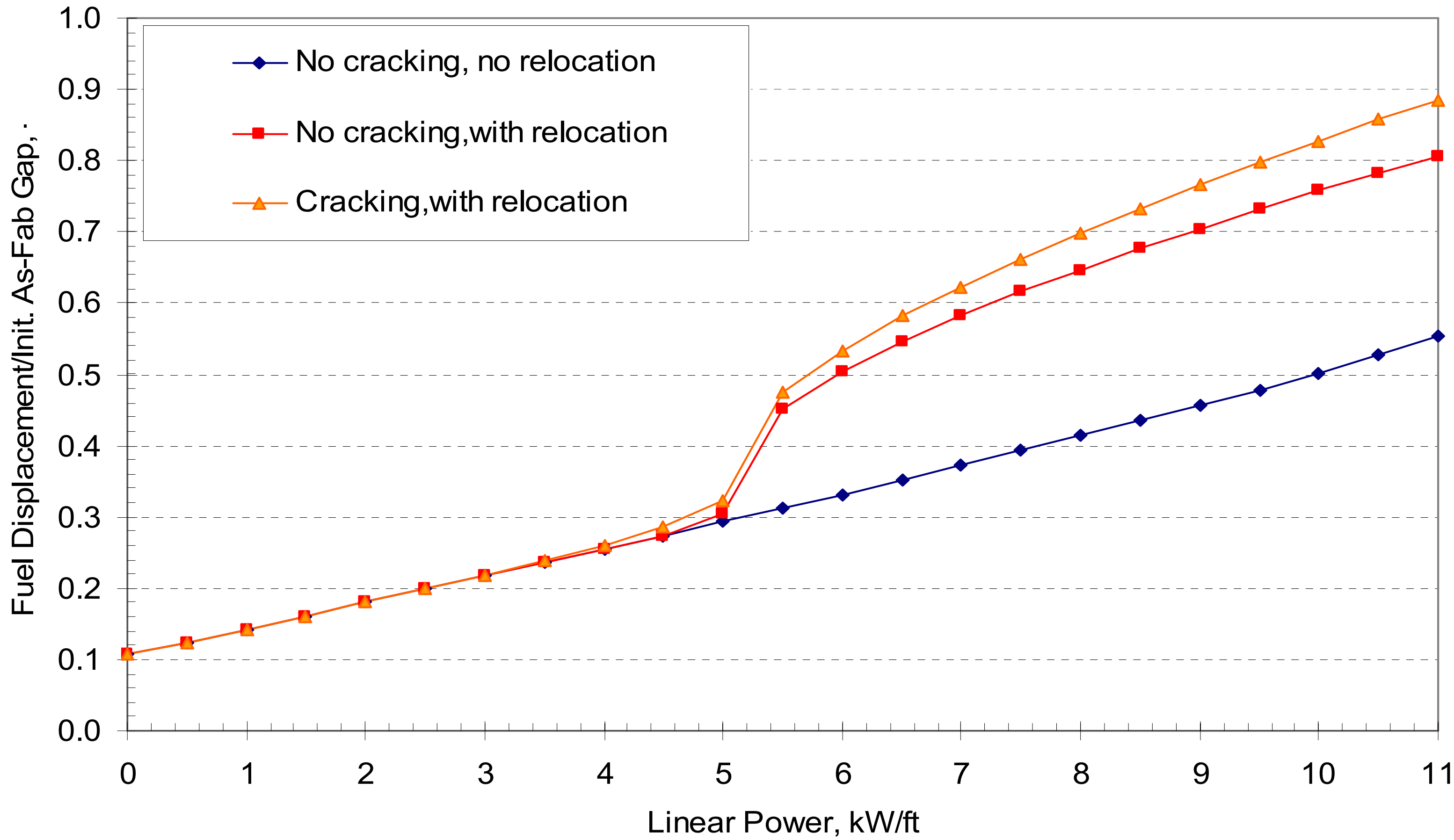
G. Zhou et al, "Westinghouse Advanced UO2 Fuel Behaviors during Power Transient," Paper 1059, 2005 Water Reactor Fuel Performance Meeting, 2-6 October, 2005, Kyoto

Thermal expansion and relocation



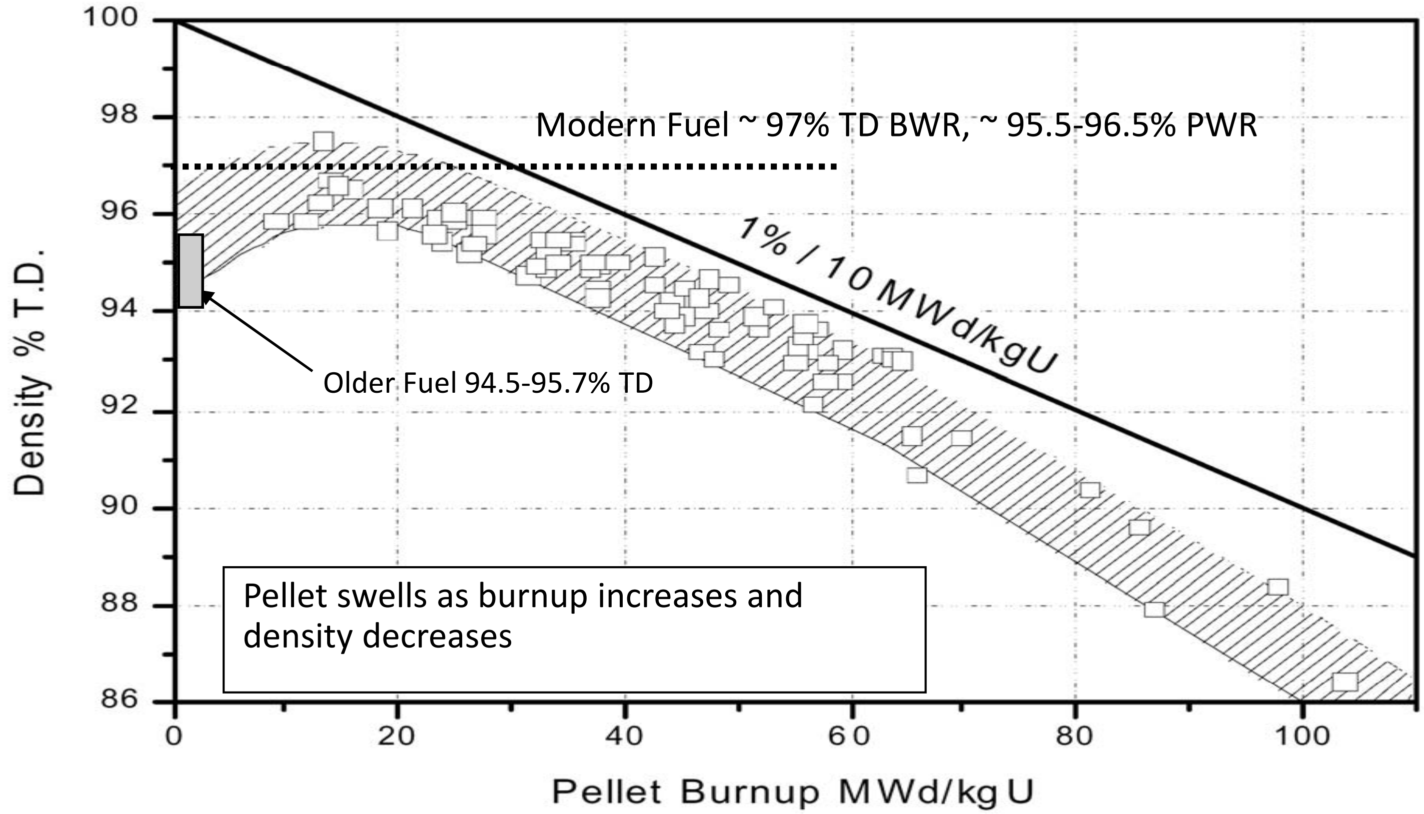
Remaining Fractional Hot Gap at BOL (i.e., Zero Exposure) Based on FALCON Analyses for 10x10 BWR and 17x17 PWR Fuel Designs

Fuel Pellet Displacement due Thermal Expansion, Relocation & Cracking as Function of Burnup and Local Linear Power for Fresh Fuel



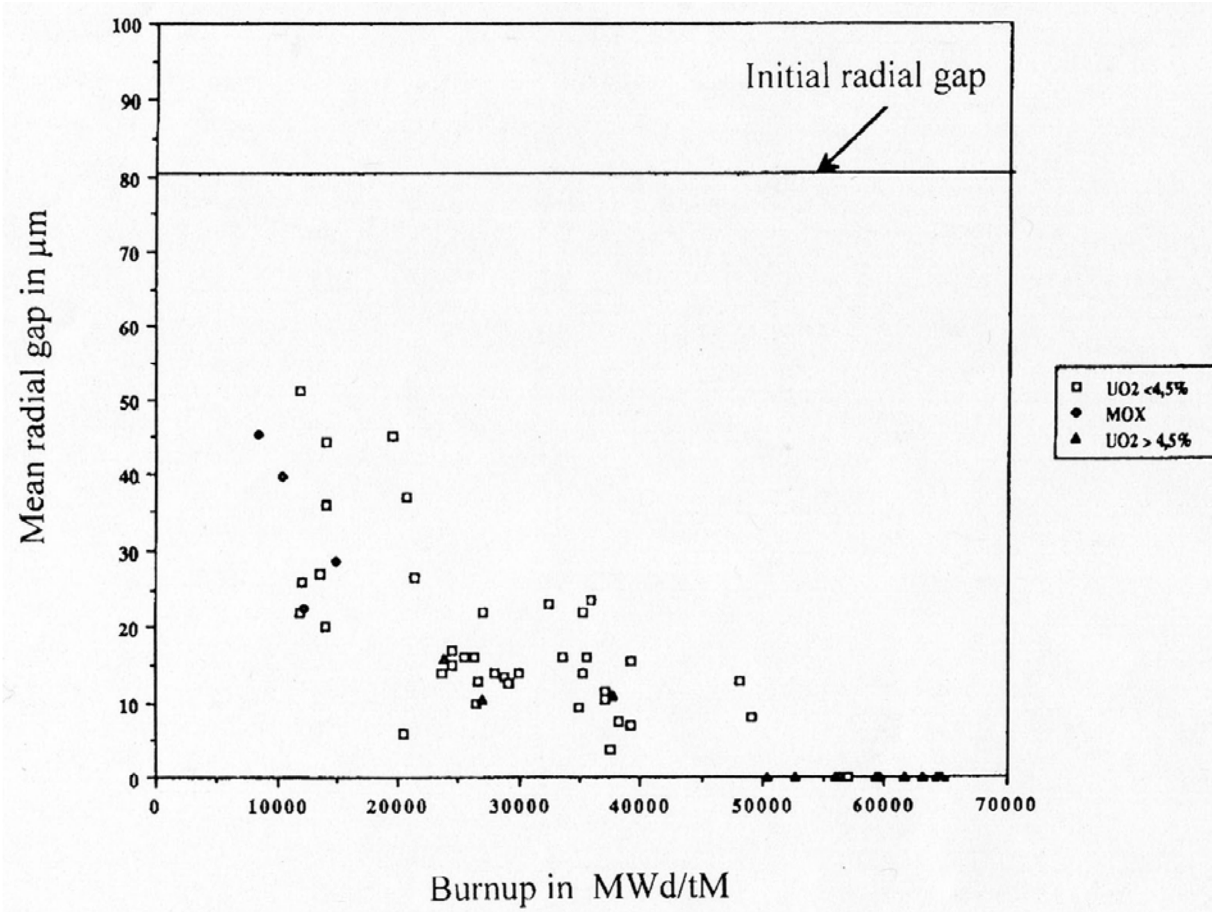
Fuel Swelling – Pellet Contraction/Expansion

Fuel Pellet Density Trend with Pellet Exposure (Matrix Swelling Rate Shown for Comparison)



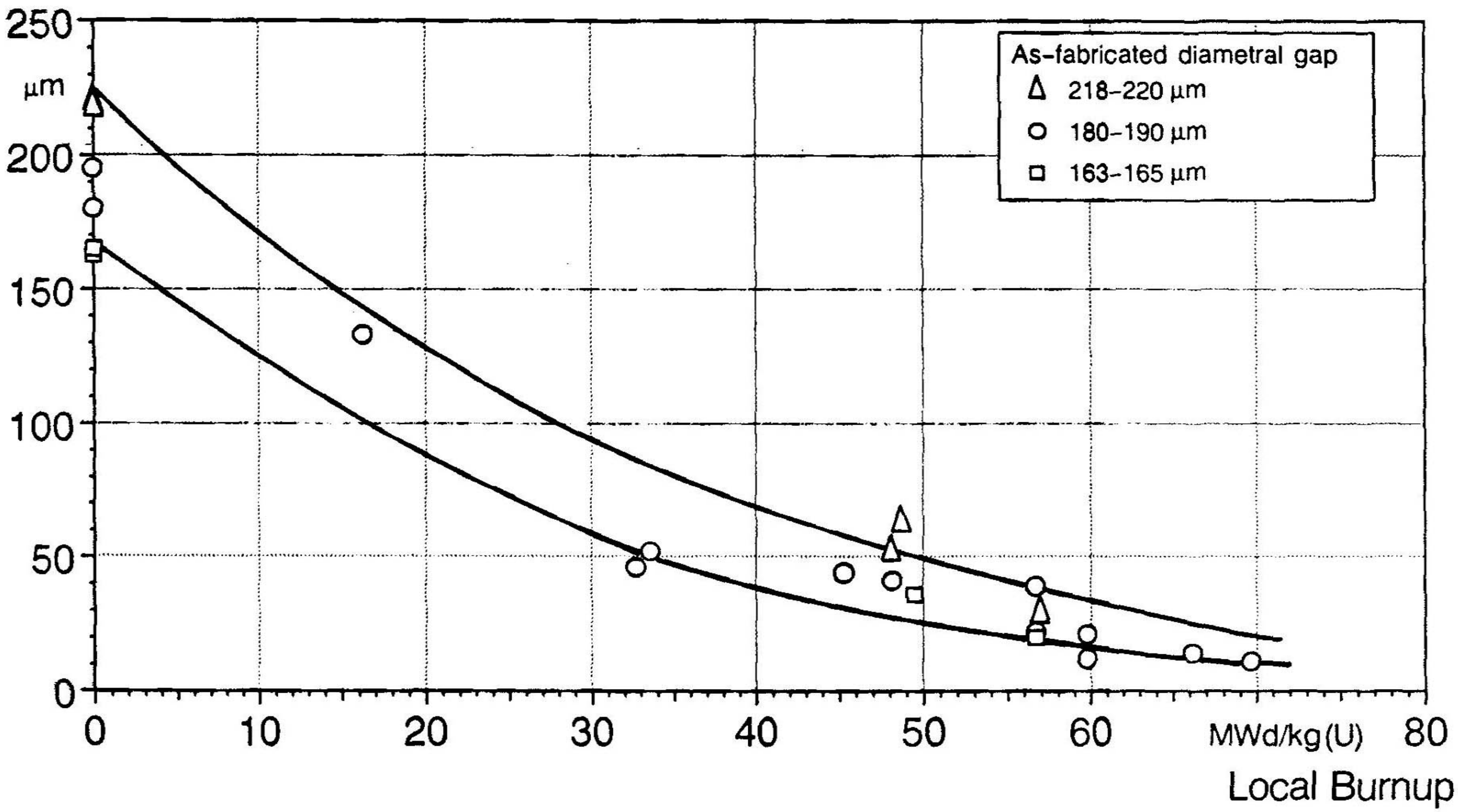
R. Manzel and C. T. Walker, “High Burnup Fuel Microstructure And Its Effect On Fuel Rod Performance,” Proceedings of the ANS 2000 International Topical Meeting on LWR Fuel Performance, Park City, April 2000

Cold Fuel-Cladding Gap (Spans 2-6) in 17x17 PWR Fuel as a Function of Rod Average Burnup

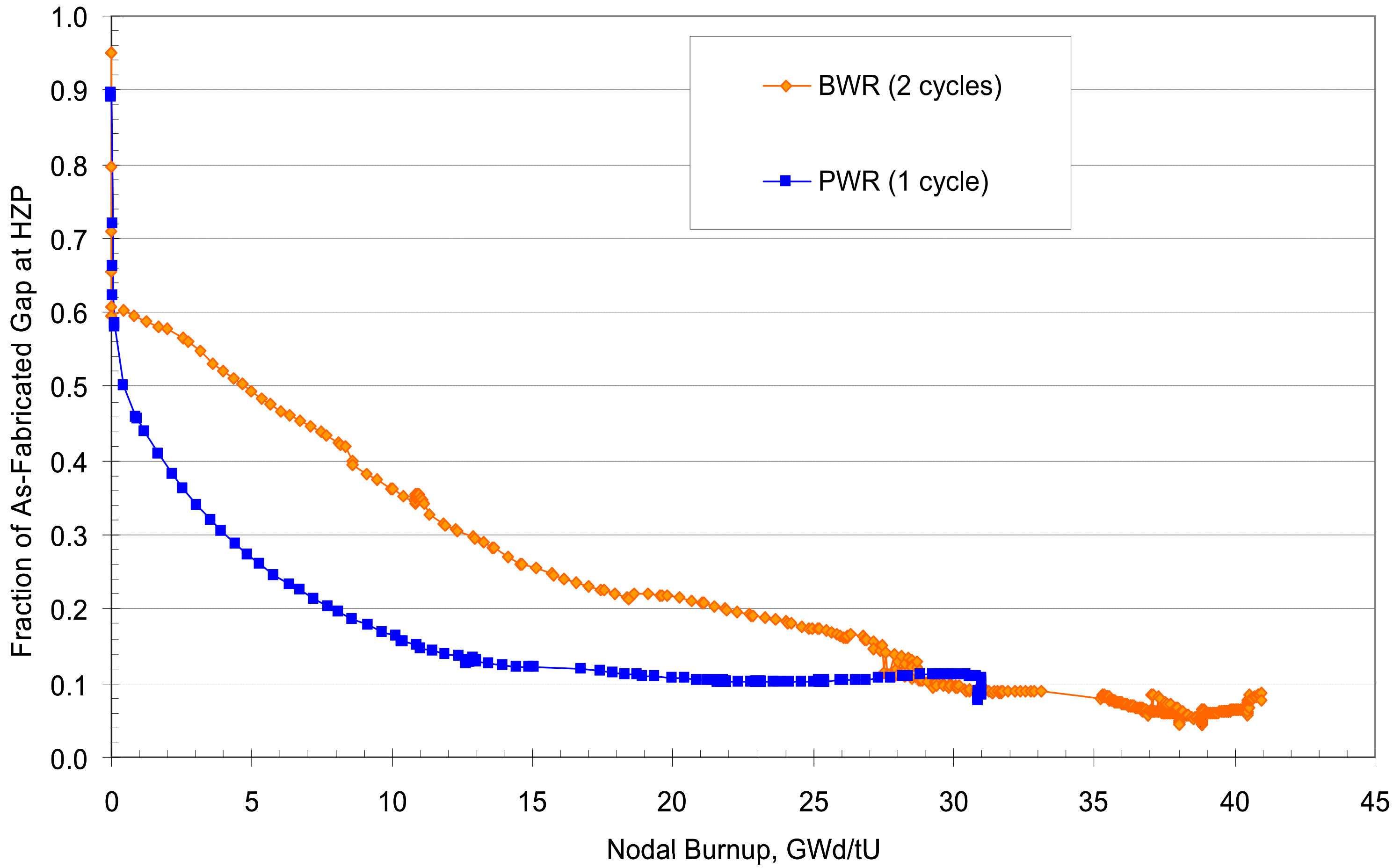


Lionel Desgranges, “Internal Corrosion Layer in PWR Fuel,” Thermal Performance of High Burn-up LWR Fuel, Seminar Proceedings, Cadarache, France, 3-6 March 1998.

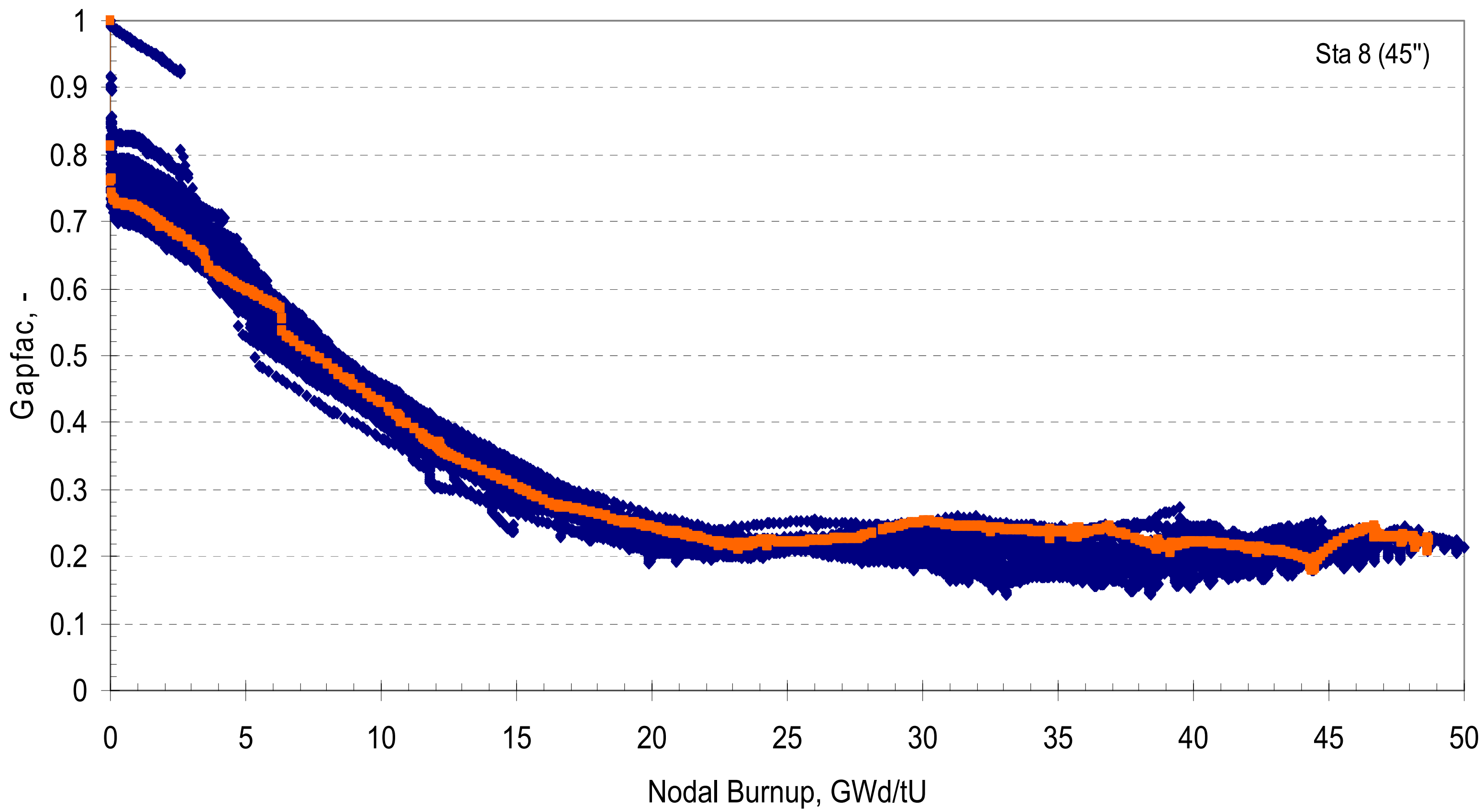
Cold Fuel-Cladding Gap in Siemens BWR Fuel



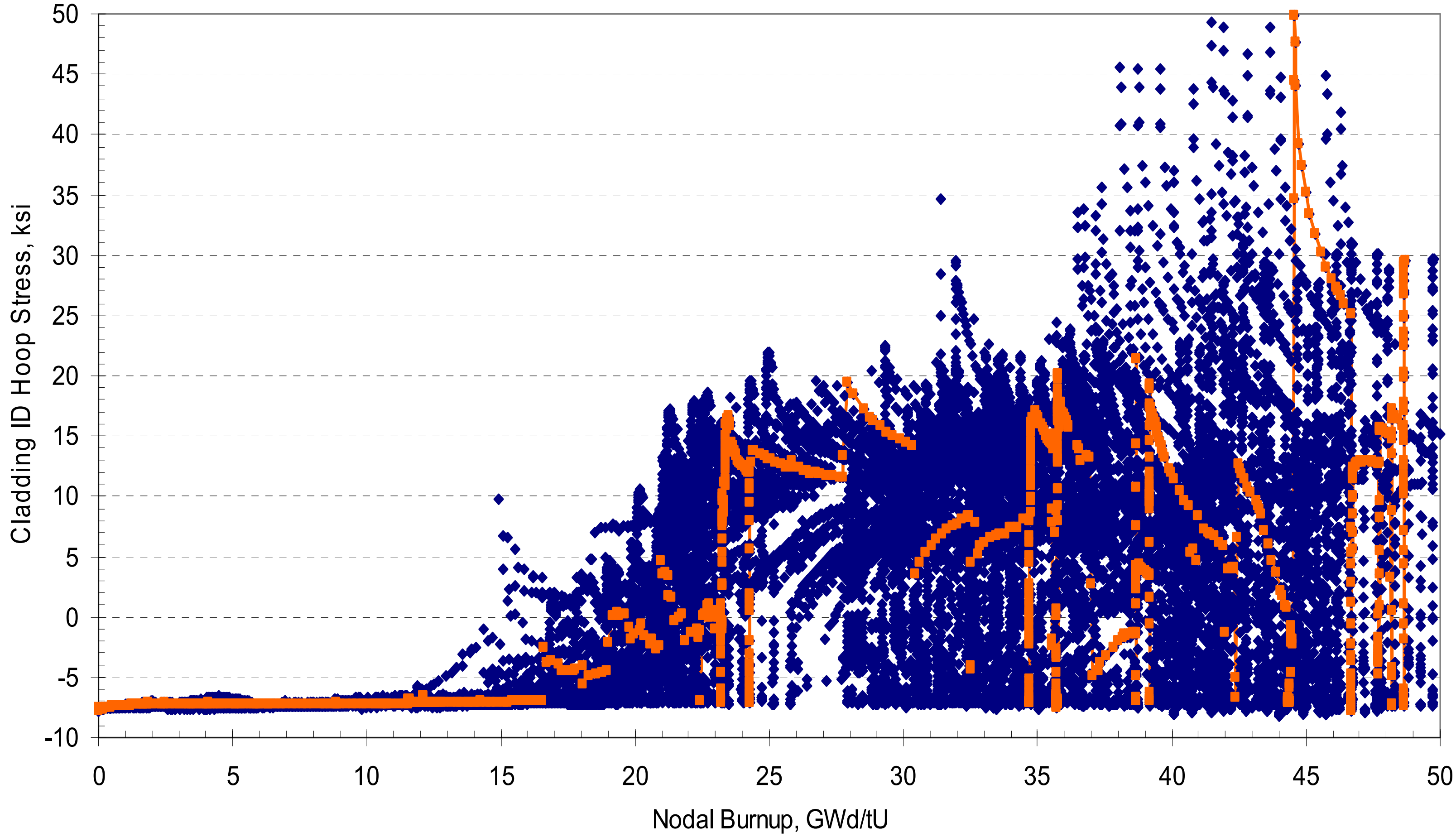
Evolution of Fuel-Cladding Gap as a Function of Nodal Burnup



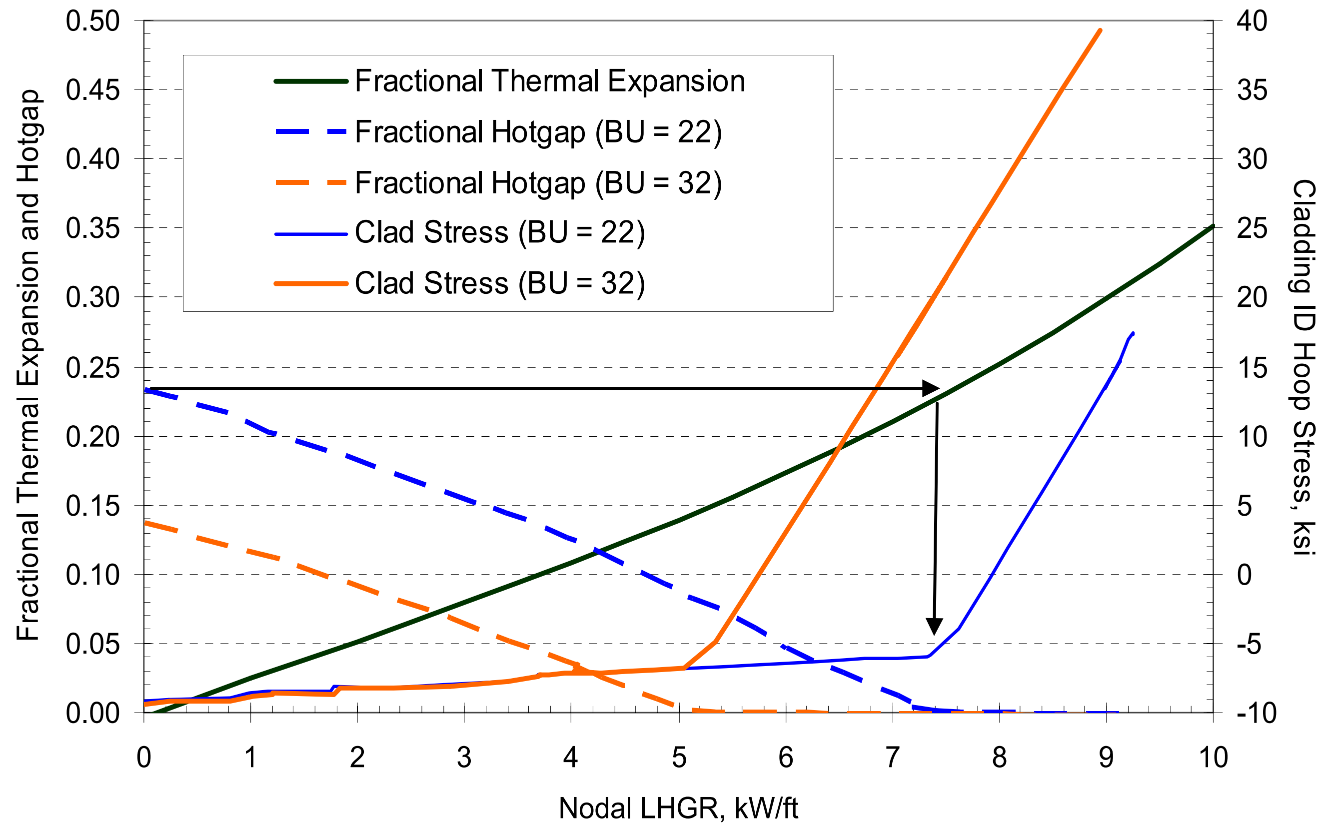
Distribution of Gaps as Function of Nodal Burnup



Distribution of Cladding Hoop Stress (RZ) as Function of Nodal Burnup



Understanding PCI
Gap Closure and Cladding Stress



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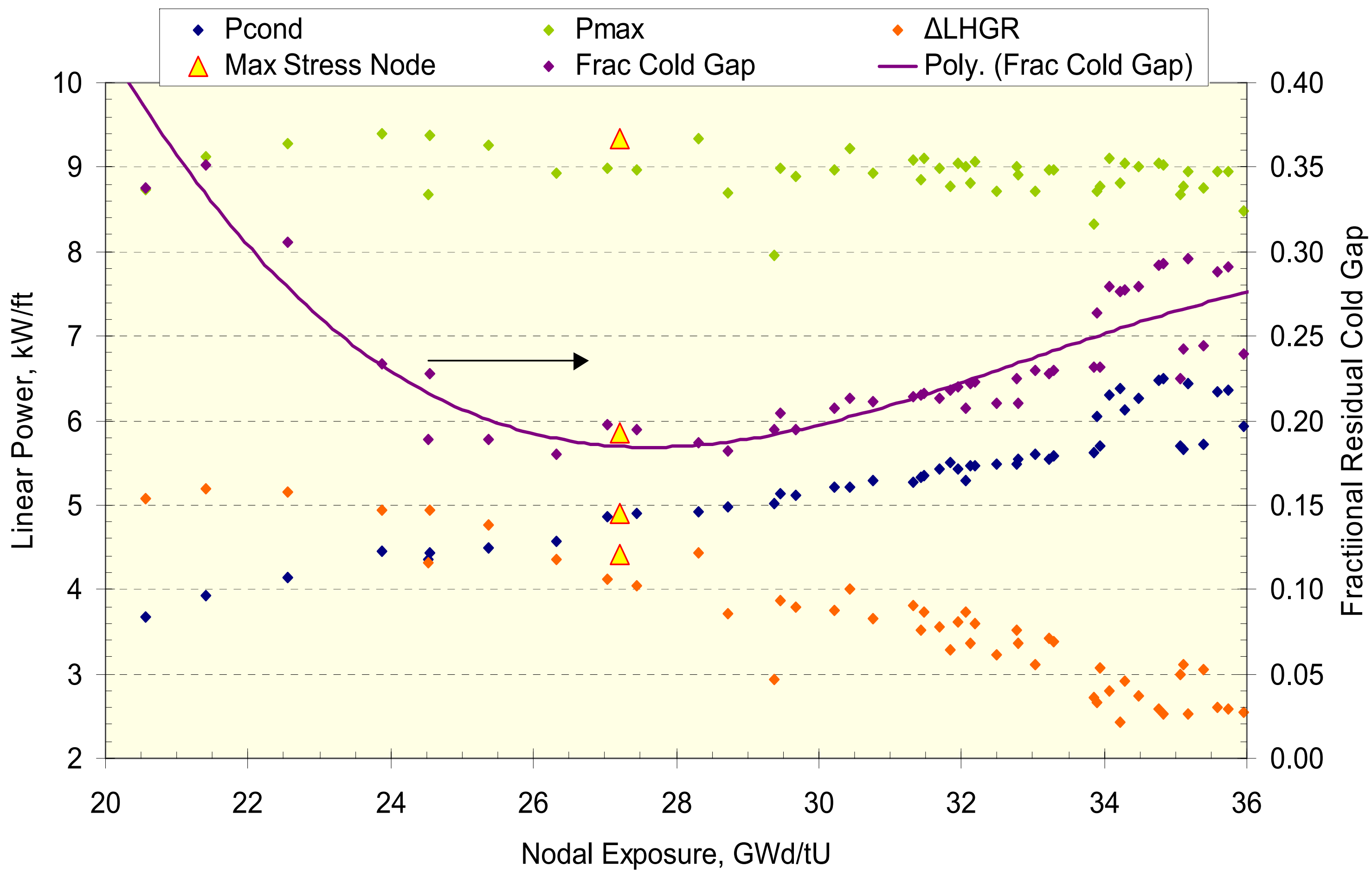
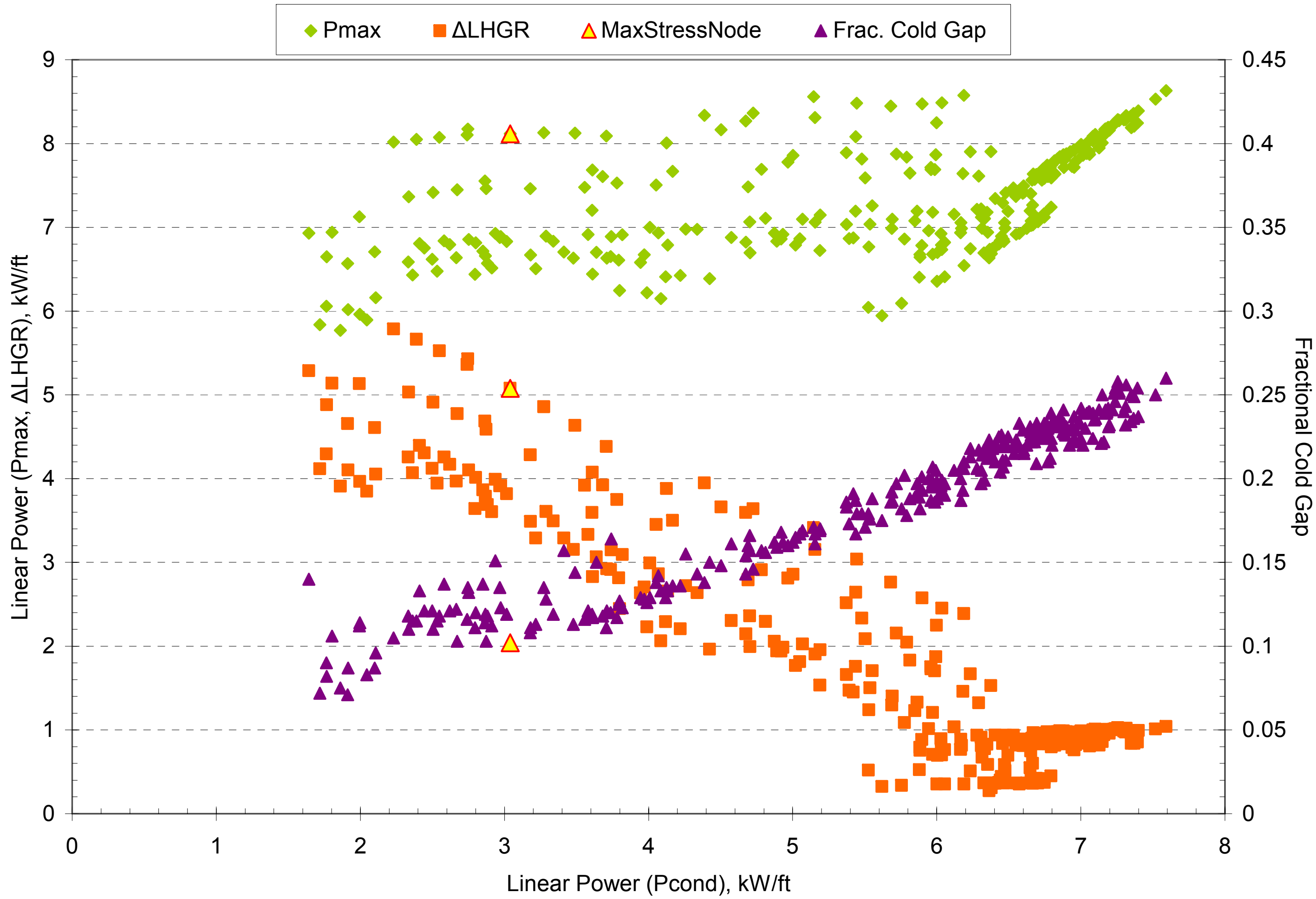
Relationship Among Burnup, Power, Gap and Cladding Stress (during a startup in a PWR)



Pmax, ΔLHGR, Frac. Cold Gap vs Pcond for 293 Peak Stress Nodes (ΔP > 0) /576 Fuel Rods, 18 Assys



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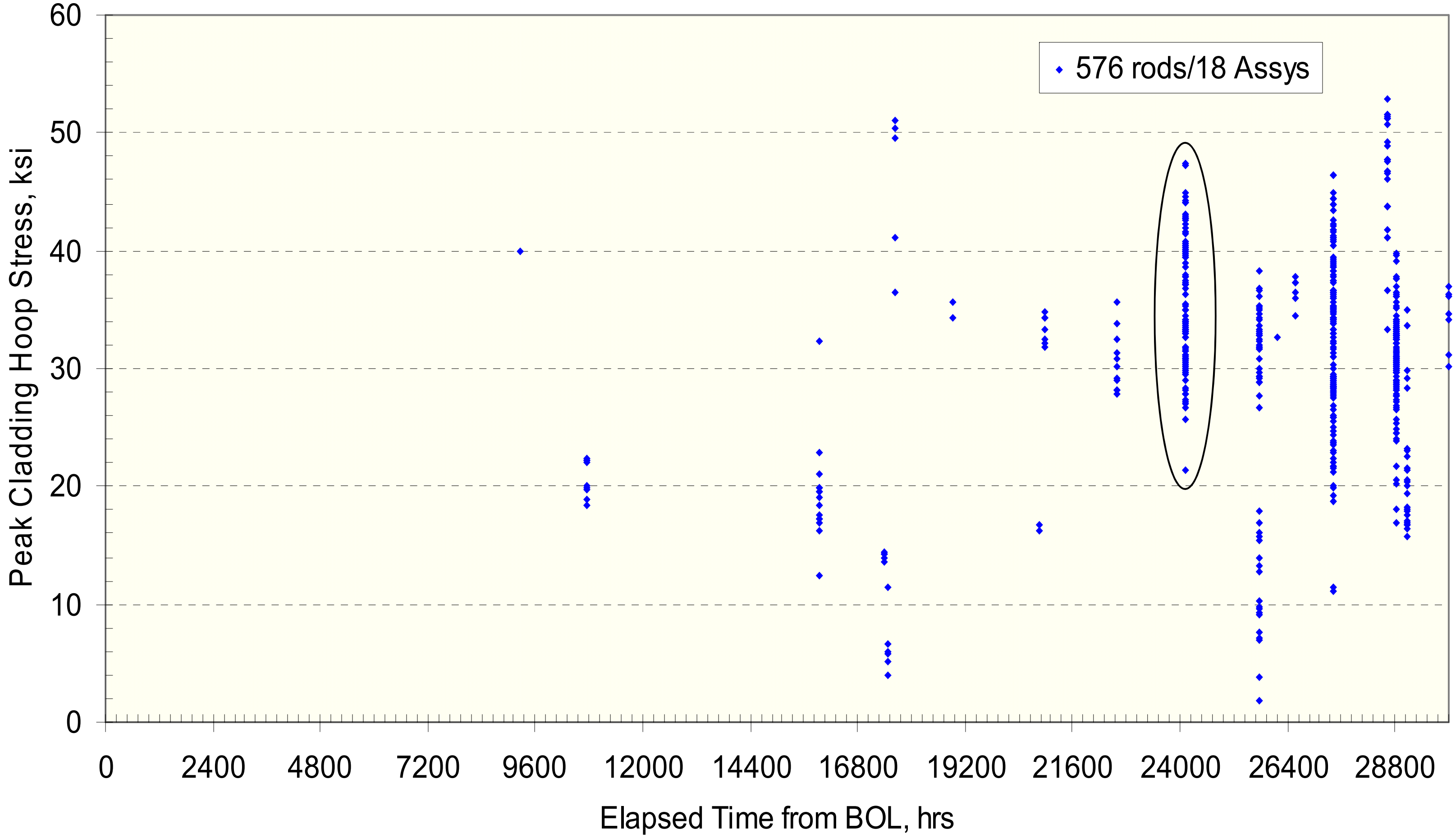
Sample Population (Peak Stress Nodes) in BWR Fuel



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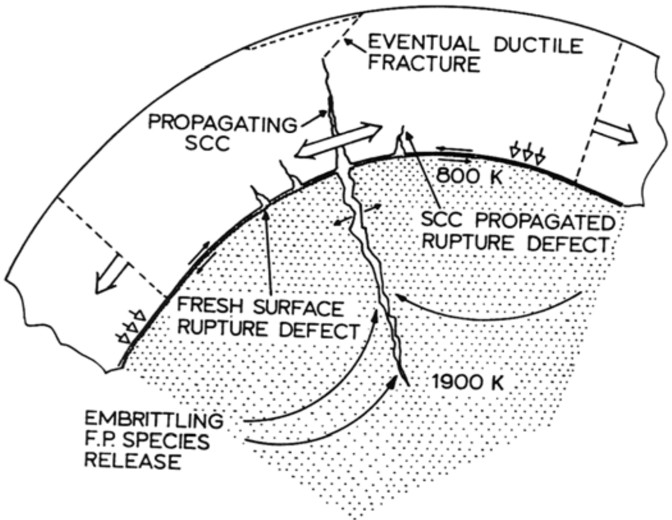
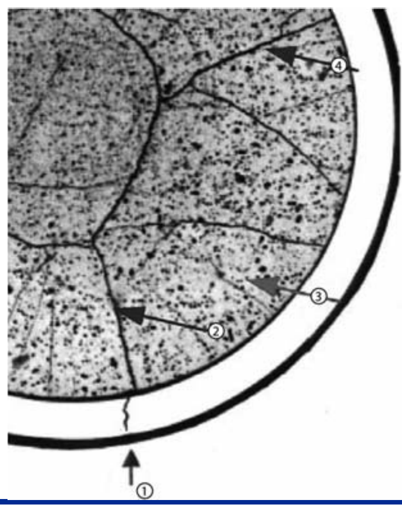
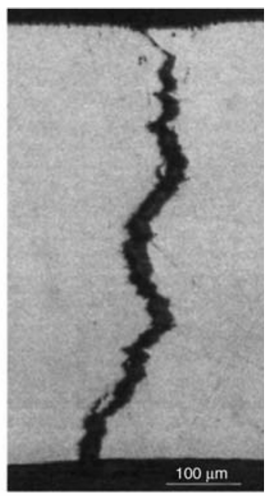
PCI Mechanism: PCMI is Pre-requisite







- Low strain failure
- Zig-zag crack pattern (tree-branching)
- Slow incubation, followed by fast propagation
- PCI is also stochastic
  - Not all tests at given nominal conditions result in failure
  - Release of fission product inventory (I) is stochastic
- Industry has developed thresholds based on failure probability in a test-reactor power ramps

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Fission Products in the Cladding Inner Surface

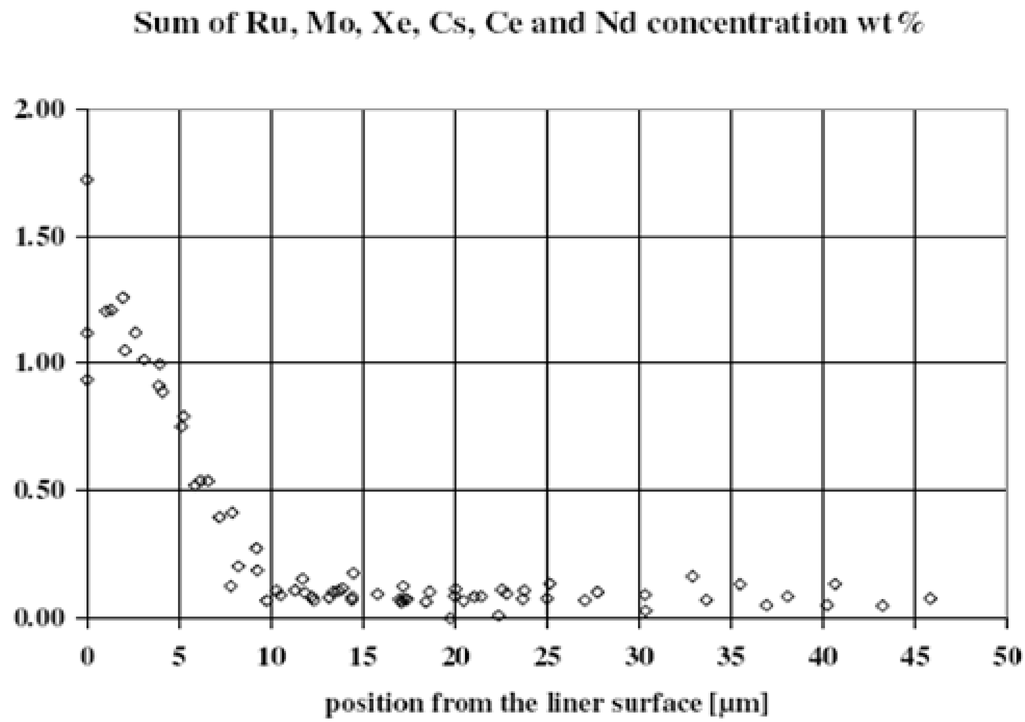


Figure 5 Sum of selected fission products measured by EPMA at the inner surface of the liner

Gunnar Lysell, Koji Kitano, David Schrire, Jan-Erik Lindbäck,
“Cladding liner surface effects and PCI,” Pellet-clad Interaction in Water Reactor Fuels,
Seminar Proceedings, OECD, Aix-en-Provence, France, 9-11 March 2004

Fission Product Release

The development of cracks in the fuel pellet provide channels for fission products like Iodine, Cesium

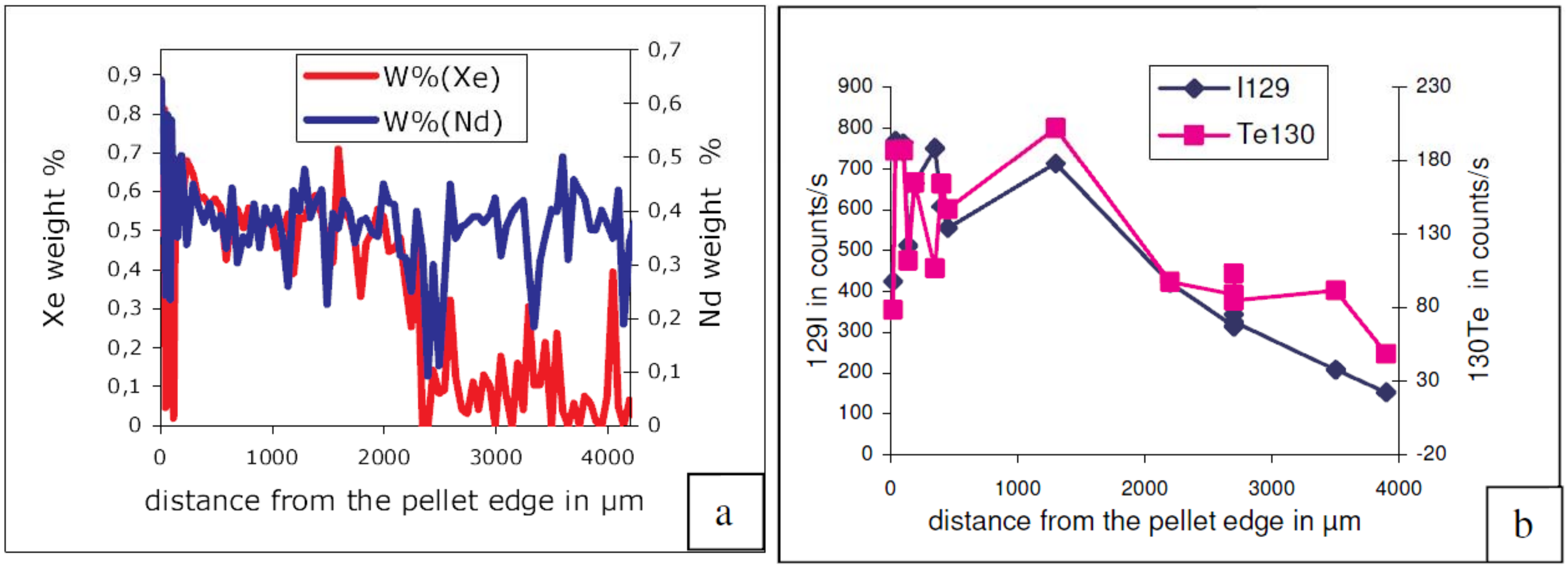
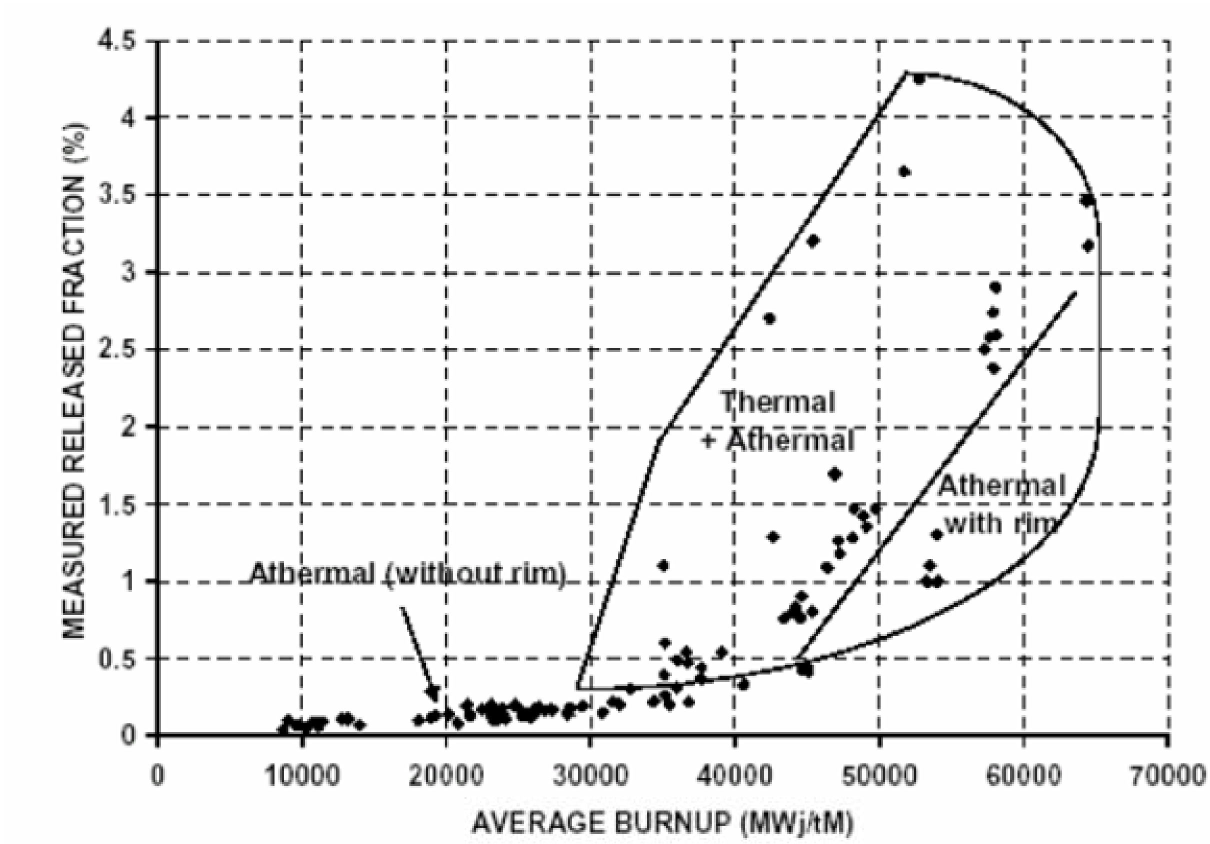


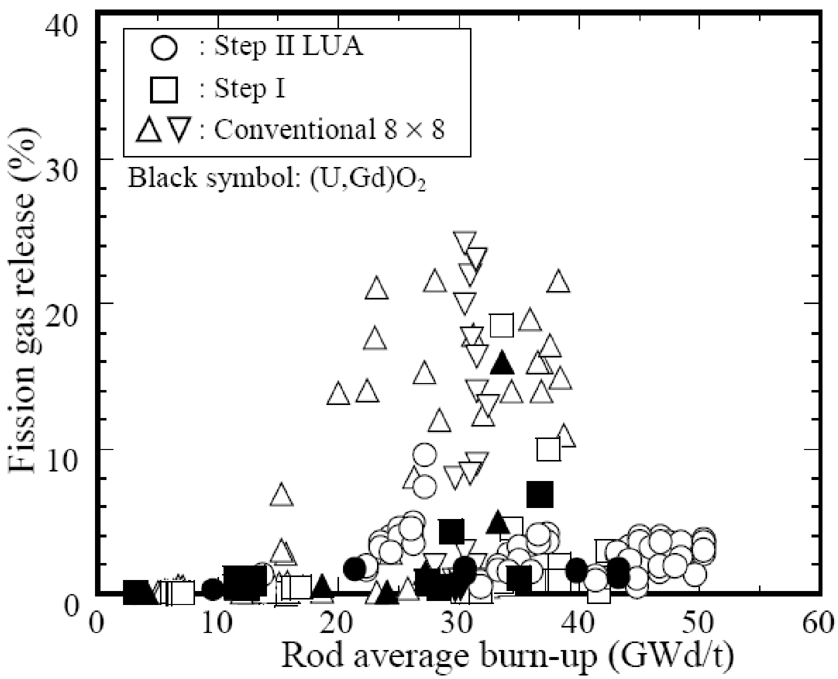
Figure 4 : EPMA quantitative concentration profile of xenon and neodymium (a) and SIMS profile of iodine and tellurium measured along the purple radius shown on figure 3.

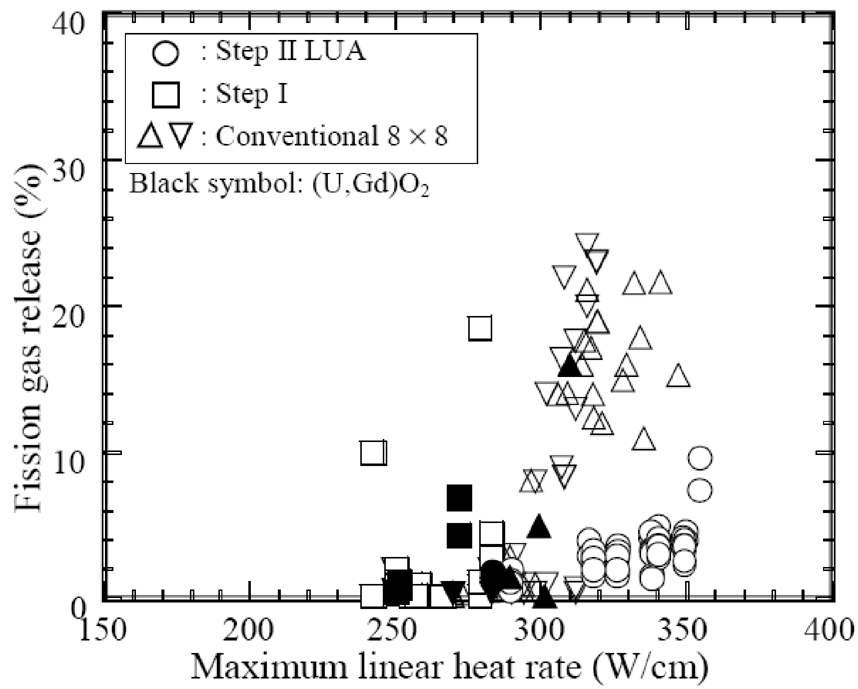
Fission Gas Release (PWR fuel)



L.C. Bernard, J. L. Jacoud, and P. Vesco, "An Efficient Model for the Analysis of Fission Gas Release." Journal of Nuclear materials 302 (2002) 125-134

Fission Gas Release (BWR fuel)





Hiroshi Sukurai et al, "Fission Gas Release and Related Behaviors of BWR Fuel under Steady and Transient Conditions," Fission Gas Behavior in Water Reactor Fuels, Seminar Proceedings, Cadarache, France, 26-29 September 2000

Fission Product Groups and Forms

Group	Title	FP or TU Elements	Oxides / Compounds
1	Noble gases	Xe, Kr	
2	Halogens	I, Br	
3	Alkali metals	Cs, Rb	M_2O
4	Tellurium group	Te, Sb, Se	MO_2
5	Barium, strontium	Ba, Sr	MO
6	Noble (Transition) metals	Ru, Rh, Pd, Mo, Tc	
7	Lanthanides	La, Zr, Nd, Eu, Nb, Pm, Sm, Pr, Y + Cm, Am	M_2O_3, MO_2
8	Cerium group	Ce, Np, Pu	M_2O_3, MO_2

Fission product element	Likely chemical state
Se, Te	Single phase chalcogenide solution $(Cs_{1-x}Rb_x)_2Se_{1-y}Te_y$ (complicated by decay Se $\rightarrow$ Br, Te $\rightarrow$ I
Br, I	Single phase halide solution $(Cs_{1-x}Rb_x)_2Br_{1-y}I_y$ (complicated by decay Br $\rightarrow$ Kr, I $\rightarrow$ Xe
Kr, Xe	Elemental state (monatomic gas)
Rb, Cs	$(Cs_{1-x}Rb_x)_2Br_{1-y}I_y$ and compounds analogous to Cs_2UO_4 , for example $(Cs_{1-x}Rb_x)_2(U_{1-y}Pu_y)O_4$ complicated by decays Rb $\rightarrow$ Sr, Cs $\rightarrow$ Ba
Sr, Ba	Oxide which can dissolve to a limited extent in the fuel and also form separate phases: $Ba_{1-x}Sr_x[Zr_{1-w-y-z}Mo_wU_yPu_z]O_3$ complicated by decays Sr $\rightarrow$ Y, Ba $\rightarrow$ La
Y, La-Eu and actinides	Oxides which dissolve in host fuel matrix
Zr, Nb	Some dissolution in host matrix
Mo, Tc, Ru, Rh, Pd	Usually single phase alloy, sometimes two phase. Some Mo can oxidize to MoO_2 and also form molybdenate compounds, e.g., Cs_2Mo_4 – $(Cs_{1-x}Rb_x)_2Mo_4$
Ag, Cd, In, Sn, Sb	Fission yield low; alloyed

Ref: Paul E. Potter, "High temperature chemistry for the analyses of accidents in nuclear reactors," Pure & Applied Chemistry, Vol. 60, No. 3, pp. 323-340, 1988.

Challenges in Multi-scale Modeling

- Multi-component system
  - Fuel matrix + Fission Products + TU
  - Cladding system
    - » Composition
    - » Structure (monolithic vs composite)
    - » Corrosion + Hydrogen pickup
    - » FP on inner surface
- Complex Thermo-mechanical and Thermo-chemical behaviors
  - Microstructure evolution (swelling, porosity, cracking, . . .)
  - Isotopic vector
- Challenge to Ab-initio Modeling
  - Substantial variation in initial conditions (e.g., pellet composition and microstructure, cladding composition and microstructure, plethora of fuel designs
  - Substantial variation in operating conditions

Conclusions

- Fuel Designs and Materials
  - Designs have evolved substantially over the last 4 decades
  - LWR Fuel Operation has evolved substantially in the last 4 decades

- Fuel Performance Codes
  - Engineering scale codes with 1-1/2 D mechanics
  - Materials properties and behavioral models are empirical
  - FREY/FALCON unique 2D axisymmetric mechanics, but materials properties and behavioral models are empirical

- Challenges in Modeling
  - Fuel-Cladding Gap, Relocation
  - PCI
  - Fission Gas Release

- Substantial variations in Fuel Designs and Operation challenge Ab-initio Modeling