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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ANATECH Corp.
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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>PWR</th>
<th>BWR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Residence time</td>
<td>3 yrs</td>
<td>4 yrs</td>
</tr>
<tr>
<td>Hot Channel Factor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Steady-state</td>
<td>1.5-2.1</td>
<td>1.8-2.2</td>
</tr>
<tr>
<td>Transient</td>
<td>2.3-2.5</td>
<td>2.3-2.5</td>
</tr>
<tr>
<td>Neutron Flux</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal (n/cm²-s)</td>
<td>4 – 6 x 10^{13}</td>
<td>3 – 5 x 10^{13}</td>
</tr>
<tr>
<td>Fast (n/cm²-s)</td>
<td>6 – 9 x 10^{13}</td>
<td>4 – 6 x 10^{13}</td>
</tr>
<tr>
<td>Burnup target (GWd/tU)</td>
<td>28 - 34</td>
<td>22-28</td>
</tr>
<tr>
<td>Fuel Types (No. Plants)</td>
<td>14 x 14 (24)</td>
<td>6 x 6 (7)</td>
</tr>
<tr>
<td></td>
<td>15 x 15 (28)</td>
<td>7 x 7 (30)</td>
</tr>
<tr>
<td></td>
<td>16 x 16 (2)</td>
<td>8 x 8 (3)           (Intro. 1973)</td>
</tr>
<tr>
<td></td>
<td>17 x 17 (6)</td>
<td>8 x 8-1 (2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>8 x 8-2 (4)</td>
</tr>
</tbody>
</table>

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

Results of Siemens Ramp Test on Fe-Enhanced Liner Cladding

Historical PWR Ramp Programs

• Over-Ramp
    » 7 failure
    » 7 failures

• Super-Ramp I (PWR)
    » 2 failures
    » 7 failures

• Trans-Ramp II
  – (1984 -1986): 6 W (17x17) fuel rods
    » 3 failures

• Trans-Ramp IV
    » 2 failures
NFI Ramp Test Program (NDA and Zr-4)

K. Goto et al, "UPDATE ON THE DEVELOPMENT OF JAPANESE ADVANCED PWR,"

Nuclear Science and Technology Interaction Program (NSTIP), ORNL, July 8, 2011 - 8 -
Mitsubishi Ramp Test (MDA and Zr-4)

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.”

Modeling – FALCON R-Z

• 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-\(\theta\) 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


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

Mesh elements approaching fuel grain size

Complexity of Nuclear Fuel Simulation

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

![Graph showing fuel displacement as a function of burnup and linear power.](image-url)
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
FALCON (ESCORE Relocation Model)

\[ \frac{\% \Delta D/D_o}{REL} = 0.8 \cdot Q \left( \frac{G_t}{D_o} \right) \left( 0.005 \cdot BU^{0.3} - 0.20D_o + 0.3 \right) \]

with:

- \[ Q = 0 \] for \[ q' < 6 \text{ kW/ft} \] (197 W/cm),
- \[ Q = (q' - 6)^{1/3} \] for \[ 6 \text{ kW/ft} < q' < 14 \text{ kW/ft} \] (459 W/cm)

where

- \( \frac{\% \Delta D/D_o}{REL} \) = 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)

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

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

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
- \( R^\infty \) = calibration parameter (= 0.006 in steady-state, 0.00755 in ramp) deciding the asymptotic limit of pellet relocation
- \( P^m_n \) = minimum contact pressure to ‘fully remove’ the relocation (implies recovery)

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)

Modern Fuel ~ 97% TD BWR, ~ 95.5-96.5% PWR

Older Fuel 94.5-95.7% TD

Pellet swells as burnup increases and density decreases

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

Cold Fuel-Cladding Gap in Siemens BWR Fuel
Evolution of Fuel-Cladding Gap as a Function of Nodal Burnup

Nodal Burnup, GWd/tU

Fraction of As-Fabricated Gap at HZP

- BWR (2 cycles)
- PWR (1 cycle)
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
Relationship Among Burnup, Power, Gap and Cladding Stress (during a startup in a PWR)
Pmax, ∆LHGR, Frac. Cold Gap vs Pcond for 293 Peak Stress Nodes 
(∆P > 0) /576 Fuel Rods, 18 Assys
Sample Population (Peak Stress Nodes) in BWR Fuel
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
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)

Fission Gas Release (BWR fuel)

### Fission Product Groups and Forms

<table>
<thead>
<tr>
<th>Group</th>
<th>Title</th>
<th>FP or TU Elements</th>
<th>Oxides / Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Noble gases</td>
<td>Xe, Kr</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Halogens</td>
<td>I, Br</td>
<td>M$_2$O</td>
</tr>
<tr>
<td>3</td>
<td>Alkali metals</td>
<td>Cs, Rb</td>
<td>MO$_2$</td>
</tr>
<tr>
<td>4</td>
<td>Tellurium group</td>
<td>Te, Sb, Se</td>
<td>MO</td>
</tr>
<tr>
<td>5</td>
<td>Barium, strontium</td>
<td>Ba, Sr</td>
<td>MO</td>
</tr>
<tr>
<td>6</td>
<td>Noble (Transition) metals</td>
<td>Ru, Rh, Pd, Mo, Tc</td>
<td>M$_2$O, MO$_2$</td>
</tr>
<tr>
<td>7</td>
<td>Lanthanides</td>
<td>La, Zr, Nd, Eu, Nb, Pm, Sm, Pr, Y + Cm, Am</td>
<td>M$_2$O, MO$_2$</td>
</tr>
<tr>
<td>8</td>
<td>Cerium group</td>
<td>Ce, Np, Pu</td>
<td>M$_2$O, MO$_2$</td>
</tr>
</tbody>
</table>

**Fission product element** | **Likely chemical state**
---|---
Se, Te | Single phase chalcogenide solution
(C$_{1-x}$Rb$_x$)$_2$Se$_{1-y}$Te$_y$ (complicated by decay Se $\rightarrow$ Br, Te $\rightarrow$ I)
Br, I | Single phase halide solution
(C$_{1-x}$Rb$_x$)$_2$Br$_{1-y}$I$_y$ (complicated by decay Br $\rightarrow$ Kr, I $\rightarrow$ Xe)
Kr, Xe | Elemental state (monatomic gas)
Rb, Cs | (Cs$_{1-x}$Rb$_x$)$_2$Br$_{1-y}$I$_y$ and compounds analogous to Cs$_2$UO$_4$, 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$_{1-w-y/2}$Mo$_w$U$_{1/2}$Pu$_{1/2}$]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$_2$Mo$_4$ $\rightarrow$ (Cs$_{1-x}$Rb$_x$)$_2$Mo$_4$
Ag, Cd, In, Sn, Sb | Fission yield low; alloyed

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