

Nuclear fuel behaviour

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Outline

- Extended introduction
 - Nuclear fuel behaviour in 40 minutes
- Solving temperature distribution (simplified)
 - Most processes are thermally driven
- Mechanical and material models
 - Cladding deformation as an example
- Fuel in-reactor behaviour
 - Simulation runs and reasons for them





Nuclear fuel





Safety barriers





Fuel behaviour

- During irradiation fuel is affected by
 - Neutron flux, pressure differential, high temperature, temperature gradient, chemically aggressive environment
- There are changes in the conditions
 - Operational transients
 - Anticipated operational occurrences
 - Accidents
- These all change fuel composition and properties



Fuel rod





Fuel rod



- Diameter approximately 1 cm, length several metres
 - Many of the phenomena are local, the conditions change axially
 - This can be used in problem simplification for analysis



Basic phenomena

- Thermal energy
- Deposited to fuel pellets by fission processes
- Radially conducted to the coolant
 - Material conductivity and gas gap conductance depend on materials, burnup, temperature, fluence et al.
 - We'll get back to this





IFA-504; Linear Rating q' = 20 kW/m





Challenge

- We're attempting to describe complex phenomena on a macroscopic scale
- For instance thermal conduction and mechanical properties depend on, e.g. the cracking of the fuel pellet, which in turn depends on the pellet internal stress state, temperature and other conditions





Fuel behaviour analysis

- Fuel behaviour analysis focuses on a single fuel rod
- Phenomena can be divided into two classes
- Steady state / normal operation
 - Effects of accumulating burnup, long-term irradiation and slow changes in the properties of the fuel
 - The production and conduction of thermal energy can be considered to be equal (d/dt=0)
 - Transients and accidents
 - Fast and strong changes in conditions, phenomena not normally encountered
 - No thermal equilibrium
- Specialized codes
 - SS: ENIGMA, FRAPCON, etc
 - Transient: FRAPTRAN, SCANAIR, etc
 - SS-codes often used in the initialization of transient codes



fragment number

with LHR

300

Crack pattern

200

Rod power (W/cm)

Phenomena in normal operation: pellet

- In normal operation, the fuel...
 - Expands due to thermal expansion
 - Cracks due to thermal stresses
 - Swells due to fission products
 - Releases gaseous products into the gas gap
 - Changes in physical and chemical composition





of pellet fragmen

umber



100





Phenomena in normal operation: cladding

- In normal operation, the cladding...
 - Is oxidized by water from outer surface
 - Creeps inward due to pressure difference
 - Takes in hydrogen, changing in properties
 - Elongates due to irradiation growth
- And, at high enough burnup...
 - Comes into contact with the pellet
 - Creeps outward with the pellet
 - Bonds chemically with the pellet





Fuel pellets after irradiation



Accidents: LOCA

- In a loss-of-coolant-accident...
 - Heat transfer is blocked and temperature in fuel and cladding rise
 - Internal pressure builds up, cladding deforms plastically, balloons, fails (> 650 °C)



- The cladding oxidizes rapidly (> 1200 °C)
 - The oxide is brittle, shatters easily
 - Zircaloy reacts with water exothermically to produce heat and hydrogen
- The pellet shatters and may be dispersed into the primary loop

^{15/04/201®} The fuel melts (> 2800 °C)





Accidents: RIA

- In a reactivity accident...
 - Sudden spike in reactivity deposits energy into the fuel extremely fast (tens of milliseconds)
 - The pellet expands rapidly due to thermal expansion, may lead to cladding failure
 - The outcome of the accident is greatly dependent on the initial state of the fuel rod (gap width, etc.)





Fuel behaviour modelling

Thermal

Temperature distribution

Fission gas release

Gap conductance

Creep

Plasticity

Cladding integrity

- Boundary conditions
 - Power distribution
 - Coolant temperature and pressure
- Solve
 - Temperature distribution
 - Mechanical deformations
 - Heat flux to coolant
 - Effects of burnup (fuel swelling, fission gas Telease, diadation growth creep, etc.)

Swelling

Thermal expansion

Heat conductivity

Mechanical

Materials



Modelling nuclear fuel behaviour



- Cladding temperature
- Pellet temperature
- Released fission gases
- Internal pressure
- PCMI
- P(Fuel failure)
- etc
- Models have been developed to describe the macroscopic effect of microscopic statistical phenomena
 - Not necessarily directly measureable
 - Models based on partially theory, partially on parameters fitted to experimental results (correlations)
- Application range and validity of the modelsi
 - Range of validity (e.g. <45 MWd/kgU), new materials, new fuel designs





Where to get information from

- No room for fuel on-line instrumentation in power reactors, but fuel behaviour in NPPs is the reason for the studies
 - Pool inspections during annual maintenance shutdowns
 - Post irradiation examinations after the irradiation
- Experimental reactors feature space for instrumentations, but do not necessarily match power reactor size or conditions (flux, temperature, pressure)
 - Several ways to compensate
 - Use of rod segments
 - Possibility for on-line instrumentation
 - Experiment to fuel damaging





Modelling fuel: Thermal element



- Fuel is regarded as a heat producing element, whose properties do not change during the modelling
 - No connection between heat transfer and mechanical solution
 - Burnup can be taken into account, but power history ignored
 - Won't need a lot of information on fuel behaviour, fast (immediate) calculation
- Common model in reactor physics, thermal hydraulics and system codes
 - Provides an approximate information on fuel temperature



Models fitted to various conditions (normal use, LOCA, RIA)

- Simulations take seconds or minutes
- In common use in fuel behaviour modelling
 - So what makes it different from the previous one...

Previous power history affects the current fuel state

Phenomena are described by models and correlations

- Fuel thermomechanical modelling radially, axial coupling via free volume gases
- Axial nodalization ~10 50 cm

Whole time in reactor modelled

Radial nodalization ~10 – 100 µm



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Modelling fuel: 1¹/₂D-fuel codes





Determining gas gap heat transfer coefficient





Modelling fuel: Finite Element Methods





- Small details inspected
 - (Part of) fuel pellet / cladding described with a fine mesh
- Accurate results on e.g. stress distribution
 - Demands precise information
 - Computationally demanding
 - Simulations take hours, days
- Taken to the logical conclusion: ab initio -modelling



Safety analyses

- Safety limits obtained primarily from experiments
- Modelling assists in evaluation and interpretation of the results
 - All things cannot be measured
- Choice of models to be used depends on
 - Resources
 - Available information
 - Application
- Conservative assumptions
 - If the models cannot describe a phenomenon (e.g. cladding ballooning during LOCA), a conservative limit is set (ballooning won't happen below 650 °C)
 - What's conservative? And when do we get too much conservatism?



Summary

- The purpose of the fuel rod is to produce thermal energy and transport it to the coolant, and to contain the radioactive substances produced in nuclear reactions
- Understanding the fuel rod performance requires knowledge on thermal, mechanical and materials behavior
- Fuel rod modeling is done with specialized computer codes that simulate thermal, mechanical and materials properties on various levels of detail



Heat transfer

mon



Normal operation: heat transfer to coolant





Solving the heat equation

$$P_{v} + \nabla(\lambda \nabla T) = c_{p} \rho \frac{dT}{dt}$$

In steady state situation:

$$\frac{dT}{dt} = 0$$

In cylinder coordinates, assuming no gradient over z or aximuthal

$$P_{v} + \nabla(\lambda \nabla T) = P_{v} + \frac{1}{r} \frac{r}{dr} \left(\lambda r \frac{dT}{dr} \right)$$

Ergo:

$$P_{\nu} + \frac{1}{r} \frac{r}{dr} \left(\lambda r \frac{dT}{dr} \right) = 0$$



Solving steady state heat

- Divergence theorem
 - Flux over a given volume's surface is a sum of sinks and sources in the volume
- In steady state we know the amount of heat produced
- No longitudal or angular gradient
- Solve the heat equations from outside in
 - Heat sources only in pellet
 - Pellet discritization



 Solution to heat exchange from cladding surface to the pellet center (cladding-coolant heat transfer part of thermal hydraulics)



Cladding temperature

- Assuming we can determine T_{co} from coolant temperature and steady state assumptions (yes we can)
- Cladding heat equation:

$$\frac{d^2T}{dr^2} + \frac{1}{r}\frac{dT}{dr} = 0 \qquad \Rightarrow \frac{dT}{dr} = \frac{a}{r}$$
$$\Rightarrow T(r) = a\ln(r) + b$$
$$\checkmark$$
• Fourier equation & power from pellet $q = \left(\lambda \frac{dT}{dr}\right)_{r_i} = \frac{P}{2\pi r_i}$

$$\Delta T = T_{ci} - T_{co} = \frac{P}{2\pi\lambda} \ln(\frac{r_o}{r_i})$$



Gap conductance





Gap conductance





Gap conductance



G.R. Horn, Babcock and Wilcox Company, Lynchburg, VA (1973) C.E. Beyer *et al.*, BNWL-1898, NRC 1 and 3 (1975)

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Temperature distribution in fuel

- This time P_v cannot be ignored
- Assuming constant P_v and λ

• BUT, P, and
$$\lambda$$
 are not constants

Solved in small radial nodes where they can be assumed constant

conductivity λ is given by

$$\lambda = 1.0789 \frac{d}{1 + 0.5(1 - d)} \lambda_{95},\tag{50}$$

 $P_{\nu} + \frac{1}{r} \frac{r}{dr} \left(\lambda r \frac{dT}{dr} \right) = 0$

 $T(r) = -\frac{P}{4\lambda}r^2 + a\ln(r) + b$

where λ_{95} is the thermal conductivity for UO₂ at 95 % of the theoretical density, and d is the as-fabricated density of pellet as a fraction from the theoretical value. The correlation for λ_{95} is

$$\lambda_{95} = \left[A + a \cdot gad + BT + f(Bu) + \left(1 - 0.9e^{-0.04Bu}\right)g(Bu)h(T)\right]^{-1} + \frac{E}{T^2}e^{-F/T}.$$
 (51)



Transient heat transfer

- Steady state yields nearparabolic temperature profile in fuel
- Transient cases where no equilibrium is a bit different





Radial temperature distribution during RIA, according to the FINIX fuel behaviour model





Radial temperature distribution during RIA, according to the FINIX fuel behaviour model



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Mechanical models



Mechanical behaviour

- Several phenomina determine the mechanical behaviour of the fuel pellet and cladding
 - Pellet ceramic material, hard & brittle
 - Cladding an alloy of Zirconium
- Some are relatively straightforward
 - Pellet swelling due to the fission products
 - Thermal sintering of the pellet
 - Cladding irradiation growth
- Others more complex
 - Gaseous bubble swelling in pellet
 - Cladding creep
- Cladding deformation as an example



On determination of the stress state of the cladding wall

- Local stress state drives the creep
 - Hence, we start by determining the stress
- For cladding without hard contact to pellets the stress is determined by the pressure differential across the cladding wall
 - Stress is given and strain changes -> creep
- If pellet pushes the cladding the strain is given and stress changes
 - Stress relaxation
- Well developed approaches using e.g. FEM
- Short detour on determining the stress analytically
 - Assume perfect geometry, isotropic properties



Stress to the cladding wall



direction



Deviatoric stress

- Part of the stress is always hydrostatic
 - In principle, the average of the stress components is just compressive and is not assumed to cause any creep

$$\sigma_{i,dev} = \sigma_i - \sigma_{hydr} = \sigma_i - (\sigma_h + \sigma_z + \sigma_r)/3$$

$$\sigma_{h,dev} = \sigma_h - (\sigma_h + 0.5\sigma_h)/3 = 0.5\sigma_h$$

$$\sigma_{z,dev} = \sigma_z - (2\sigma_z + \sigma_z)/3 = 0$$

- No creep in axial direction!
 - This is why usually irradiation growth is noted only in axial direction
- But, this treatment for thin tubes (wall thickness less than tenth of diameter



Thick walled tube

- Stress distribution (inside the wall) must also taken into account
 - Also radial stresses
 - Often mid-wall stresses calculated

$$\sigma_{h} = A + \frac{B}{r^{2}} \qquad A = \frac{r_{i}^{2}P_{i} - r_{o}^{2}P_{o}}{r_{o}^{2} - r_{i}^{2}}$$

$$\sigma_{z} = A \qquad B = \frac{(P_{i} - P_{o})r_{o}r_{i}}{r_{o}^{2} - r_{i}^{2}}$$

- Main conclusions the same, no creep in axial direction
- BUT, hoop stress and deviatoric hoop stress are not zero at the same pressure differential!



Deviatoric hoop stress versus hoop stress

- If internal and external pressures are the same, mid-wall there will be hoop stress
 - However, it is equal to hydrostatic stress, ergo no creep
- However we see that, using thick wall approximation, the hoop stress is not linearly relative to deviatoric hoop stress at low stresses!





Actual experimental results may differ

We must remember the previous discussion is theoretical



[Mathew, M.D., Ravi, S., Vijayanand, V.D., Latha, S., Dasgupta, A., Laha, K., 2014. Biaxial creep deformation behavior of Fe–14Cr–15Ni–Ti modified austenitic stainless steel fuel cladding tube for sodium cooled fast reactor. Nucl. Eng. Des. 275, 17-22].





Cladding deformation as an example

An idealised constant stress thermal creep curve (ABCDE) is illustrated in fig. 1(a). The total strain to fracture (ϵ_E) is given by:

 $\epsilon_{\rm E} = \epsilon_{\rm e} + \epsilon_{\rm p} + \epsilon_{\rm R} + \epsilon_{\rm C} + \epsilon_{\rm T} \; , \label{eq:electric}$

where ϵ_e and ϵ_p are the elastic and plastic loading strains, ϵ_R is the anelastic or recoverable strain (assumed here to be introduced only during the primary or transient creep stage), ϵ_C is the steady state creep strain and ϵ_T is the tertiary creep strain. If, however, the stress is removed at C (time t_C) and the temperature maintained constant, the elastic (ϵ_e) and anelastic (ϵ_R) strains recover as indicated by curve CFG, the residual plastic strain being given by ($\epsilon_p + \epsilon_C$).

Journal of Nuclear Materials **65** (1977) 157-173 D. Harries, Irradiation creep in non-fissile metals and alloys



Instantenous reversible deformation (elastic and thermal)

Given the internal pressure P, the outside (coolant) pressure P_o , and the cladding inner and outer radii, R_{ci} and R_{co} , the hoop stress σ_{θ} and the axial stress σ_z are obtained as

$$\sigma_{\theta} = \frac{R_{ci}P - R_{co}P_o}{R_{co} - R_{ci}},\tag{27}$$

$$\sigma_z = \frac{R_{ci}^2 P - R_{co}^2 P_o}{R_{co}^2 - R_{ci}^2}.$$
(28)

The hoop, axial and radial strains are connected to the stresses through relations

$$\epsilon_{\theta} = \frac{1}{E} (\sigma_{\theta} - \nu \sigma_z) + \epsilon_{\rm th}, \qquad (29)$$

$$\epsilon_z = \frac{1}{E} (\sigma_z - \nu \sigma_\theta) + \epsilon_{\rm th}^{\rm z}, \tag{30}$$

$$\epsilon_r = -\frac{\nu}{E}(\sigma_\theta + \sigma_z) + \epsilon_{\rm th},\tag{31}$$



Plastic deformation

 Often used (simplified) assumption is that below yield stress there is only elastic strain, above it (rate dependent) plastic strain



Figure 2.7 Typical Isothermal Stress-Strain Curve



Irradiation growth

- Irradiation growth is volumeconserving deformation that happens under irradiation
 - No stress needed
 - Assumed to be additive to creep
- Decreases the hcp structure in basal pole direction, increases in prismatic pole direction
 - Cladding tubes formed intentionally so that the basal poles are preferentially in radial direction
 - Diameter decrease, length increase



Basal pole

pole



Creep

- Experimental observations
- Mechanisms behind creep deformation
- Modelling of creep



Experimental observations

- Thermal creep in three stages
 - Primary creep with diminishing creep rate
 - Secondary creep with stationary creep rate
 - Tertiary creep with increasing creep rate ending in a break
- Irradiation increases the numbers of various defects
 - Accelerated creep
 - Accelerated material hardening
- At high temperature thermal creep dominates



Figure from V. Fidleris, The irradiation creep and growth phenomena, JNM **159** (1988) 22-42



Experimental observations

- At low stress creep rate is relative to the stress
- At medium stress creep rate is approx stress to power of 5
- At high stress the relation is exponential
 - "Power law breakdown"



Figure from T.A. Hayes and M.E. Kassner, Creep of Zirconium and Zirconium Alloys, Metallurgical and Materials Transactions A **37A** (2006) 2389-2396



Mechanisms of creep

- Thermal creep
 - Dislocation creep (or climb and glide)
 - Diffusional creep
 - Nabarro-Herring and Coble creep
- Irradiation creep
 - Stress-induced preferential nucleation of loops (SIPN)
 - Stress-induced preferential absorption (SIPA)
 - Climb and glide assisted by irradiation defect formation
- Different mechanisms work at parallel
 - Creep rate determined by the fastest mechanism



Figure from D. Knorr and M. Notis, Deformation mechanism mapping of alpha-Zr and Zircaloy-2, JNM **56** (1975) 18



Mechanisms of creep Thermal creep: Dislocation creep

- Dislocations (deviation from a perfect lattice structure) either exist or are created by the stress
- Dislocations glide through a lattice plane driven through stress
- Glide is arrested by an obstacle
 - Climbing over obstacle takes time / energy
 - Pile-up of dislocations





- Also opposite dislocations attract each other
 - Dislocation annihilation





Mechanisms of creep Thermal creep: Diffusional creep

- At high temperature and low stresses atom diffusion by way of vacancies a rate determining mechanism
 - Vacancies flow from one grain face to other changing the form of the grain
 - Nabarro-Herring creep
- At lower temperatures grain boundary diffusion dominates
 - Coble creep
- Creep rate relative to stress, depends on grain size



Mechanisms of creep Irradiation creep

- Stress-Induced Preferential Nucleation of Loops
 - Loops nucleate on preferred planes depending on stress
 - Basically deforms to the direction to tensile stress
- Stress-Induced Preferential Absorption and Preferred Absorption Glide
 - Atoms are transferred from one plane to another due to stress (SIPA)
 - Dislocations glide (PAG)
- ...there are several other possible mechanisms also
 - See e.g. G. Was, Fundamentals of Radiation Materials Sceince 2007



Can known mechanisms be attributed to the experimental observations?

- SIPN accounts best the primary creep behaviour
 - Cannot explain steady state creep
- SIPA most likely explanation for in-reactor creep
 - Very little thermal creep at reactor temperatures and stresses



Phenomenological models

- Various formulations for in-reactor creep exists
- In general phenomenological
 - Correlations derived from experiments
 - Information from mechanistic understanding of creep necessarily partially lost
 - Parameters fitted to particular cladding types
 - In general vendors have more data (and thus better predictions) for their own cladding types even if the models may be quite simple



Creep models

- Phenomenological creep models
 - May separate thermal and irradition creep OR just assume in-reactor conditions
 - Usually separate the effects of stress, temperature, flux and fluence as well as material parameters
 - Primary creep may or may not be taken explicitly into account

 $\dot{\varepsilon} = f(\sigma)f(T)f(\phi)f(t)f(\chi)$

Some examples to follow



MATPRO creep model

$$\dot{\varepsilon} = K(\sigma + Be^{C\sigma})\phi t^{-0.5}e^{-\frac{Q}{RT}}$$

- Creep rate for in-reactor creep
- Low and high stress responses
- Linear flux dependence
- Constantly lowering creep rate
 - "Primary creep" and radiation hardening taken into account by it
- Arrhenius function for temperature dependence



Model evolution: Creep model by Matsuo 1987

- For the thermal creep of Zircaloy-4
- Separates primary and secondary creep
- Primary creep magnitude and rate relative to secondary creep rate
- Hyperbolic sin used to model both low and high stress regions
 - *n*=2 has no physical explanation but improves the fitting
- E is the elastic modulus

$$\varepsilon_{tot} = \varepsilon_p^s \left(1 - e^{-C\sqrt{\dot{\varepsilon}_{sec} \cdot t}} \right) + \dot{\varepsilon}_{sec} \cdot t$$
$$\varepsilon_p^s = B(\dot{\varepsilon}_{sec})^b$$
$$\langle E \rangle = (a \cdot \sigma)^n = 0$$

$$\dot{\varepsilon}_{th} = A\left(\frac{E}{T}\right) \left[\sinh\left(\frac{a\cdot\sigma}{E}\right)\right]^n e^{-\frac{Q}{RT}}$$



Model evolution: Creep model by Limbäck and Andersson 1996

$$\varepsilon_{tot} = \varepsilon_p^s \left(1 - e^{-52\sqrt{\dot{\varepsilon}_{sec} \cdot t}} \right) + \dot{\varepsilon}_{sec} \cdot t$$

$$\varepsilon_p^s = B(\dot{\varepsilon}_{sec})^b [2 - \tanh(D\dot{\varepsilon}_{sec})]^d$$

$$\dot{\varepsilon}_{sec} = \dot{\varepsilon}_{th} + \dot{\varepsilon}_{irr}$$

$$\dot{\varepsilon}_{th} = A\left(\frac{E}{T}\right) \left[\sinh\left(\frac{a\sigma}{E}\right)\right]^n e^{-\frac{Q}{RT}}$$

$$a = a_1 \left\{ 1 - a_2 \left[1 - e^{-a_3(\phi t)^{a_4}}\right] \right\}$$

$$\dot{\varepsilon}_{irr} = C(10^4 \phi)^{c_1} \sigma^{c_2}$$



Changes in conditions accounted by the strain hardening law



- Creep curves determined from single stress experiments can be used in transient cases assuming the accumulated strain is invariable when conditions change
- Lucas and Pelloux showed in 1981 that strain hardening applies to Zirc alloys in some conditions
- Adopted to most integral fuel codes
- Conceptually simple



Strain hardening law

- Load drops and reversals not well accounted by strain hardening rule
- Also stress relaxation
 - Under forced displacement, sample stress relaxes with time
 - Sort of inverse of creep







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Fuel behaviour



Fuel behaviour

- Fuel behaviour code
 - Common solution scheme
- Applications
 - Ensuring safe use of fuel
 - Coupled safety analysis



Fuel behaviour code: FINIX as an example

- Thermomechanically coupled solution
- Models and correlations validated
- Whole time in reactor simulated





YVL B.4.1 & B.4.2 (general)

401. The integrity of nuclear fuel shall be ensured during its <u>operation</u>, handling, transport, long-term storage and final disposal.

406. In determining the design criteria for nuclear fuel, the physical, chemical and mechanical phenomena that affect the durability of the nuclear fuel during operational and accident conditions shall be comprehensively analysed. The analyses shall cover all design basis scenarios.

409. Irradiation-induced changes that affect nuclear fuel properties shall be taken into account in determining the limits for safe use of the fuel, including the effects on the final disposal of spent nuclear fuel. Burn-up limits to be applied to nuclear fuel shall be presented, and they shall be based on experimental data.



YVL B.4.3 (normal operation)

412. In normal operational conditions, the nuclear fuel shall fulfil the following conditions:

- <u>No melting</u> shall occur in fuel pellets.
- <u>Cladding temperature</u> shall not substantially exceed coolant temperature.
- Fuel rod cladding shall not collapse.
- <u>The internal pressure</u> of a fuel rod shall not increase to the extent that cladding deformations caused by it would negatively affect the heat transfer between fuel pellets and coolant (no liftoff occurs).

413. Deformations in the fuel assembly and control rod components shall remain minor Assembly level is not considered in this lecture.

414. The probability of a fuel failure caused by <u>mechanical interaction</u> <u>between fuel pellet and cladding shall</u> be extremely low.



YVL B.4.4 (anticipated operational occurrences)

415. In anticipated operational occurrences:

• <u>No melting</u> shall occur in fuel pellets.

• Adequate cooling of the cladding shall be ensured. (...) Thermal hydraulic analyses not considered in this lecture.

• The probability of fuel failure caused by <u>mechanical interaction between fuel</u> and cladding shall be extremely low.







Normal operation, effect of linear heat rate

- Burnup of nuclear fuel is limited by the degradation of cladding material properties (oxidation, hydriding), pellet swelling, fission gas release, formation of high burnup structure in the pellet, enrichment
- Performance in transients
- To reach a certain burnup safely, how to distribute the linear heat rate between cycles?

409. Irradiation-induced changes that affect nuclear fuel properties shall be taken into account in determining the limits for safe use of the fuel, including the effects on the final disposal of spent nuclear fuel. <u>Burn-up limits</u> to be applied to nuclear fuel shall be presented, and they shall be based on experimental data.


Case 1: constant LHR





Case 2: low LHR for 3rd cycle





Case 3: high LHR for 3rd cycle





Multiphysics applications



TECHNOLOGY FOR BUSINESS

 $\sqrt{2}$

<u>.</u>