Physical Principles and Computational Codes for Fuel Behaviour Modelling

Lecture 9.3

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Joint ICTP-IAEA Workshop on

The Training in Basic Radiation Materials Science and its Application to Radiation Effects Studies and Development of Advanced Radiation-Resistant Materials

Trieste, November 10-21, 2008

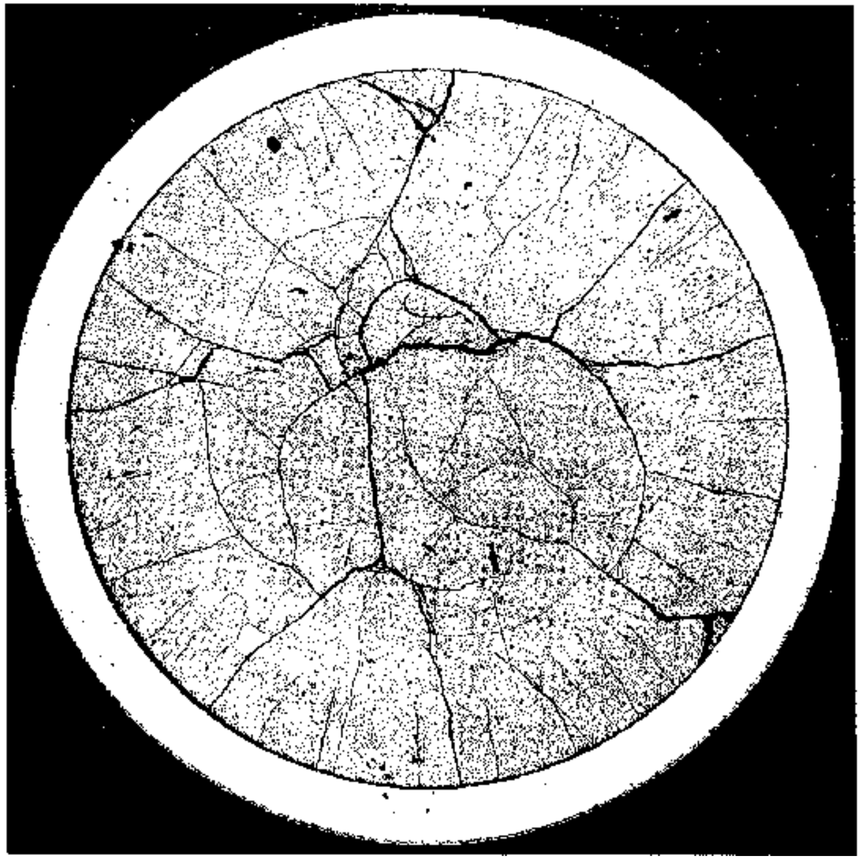
Overview

- Application of fuel modelling codes
- Essential elements
  - temperature calculations
  - fission gas release
  - dimensional changes and mechanical loads
- Overview of codes

Application of Fuel Performance Codes

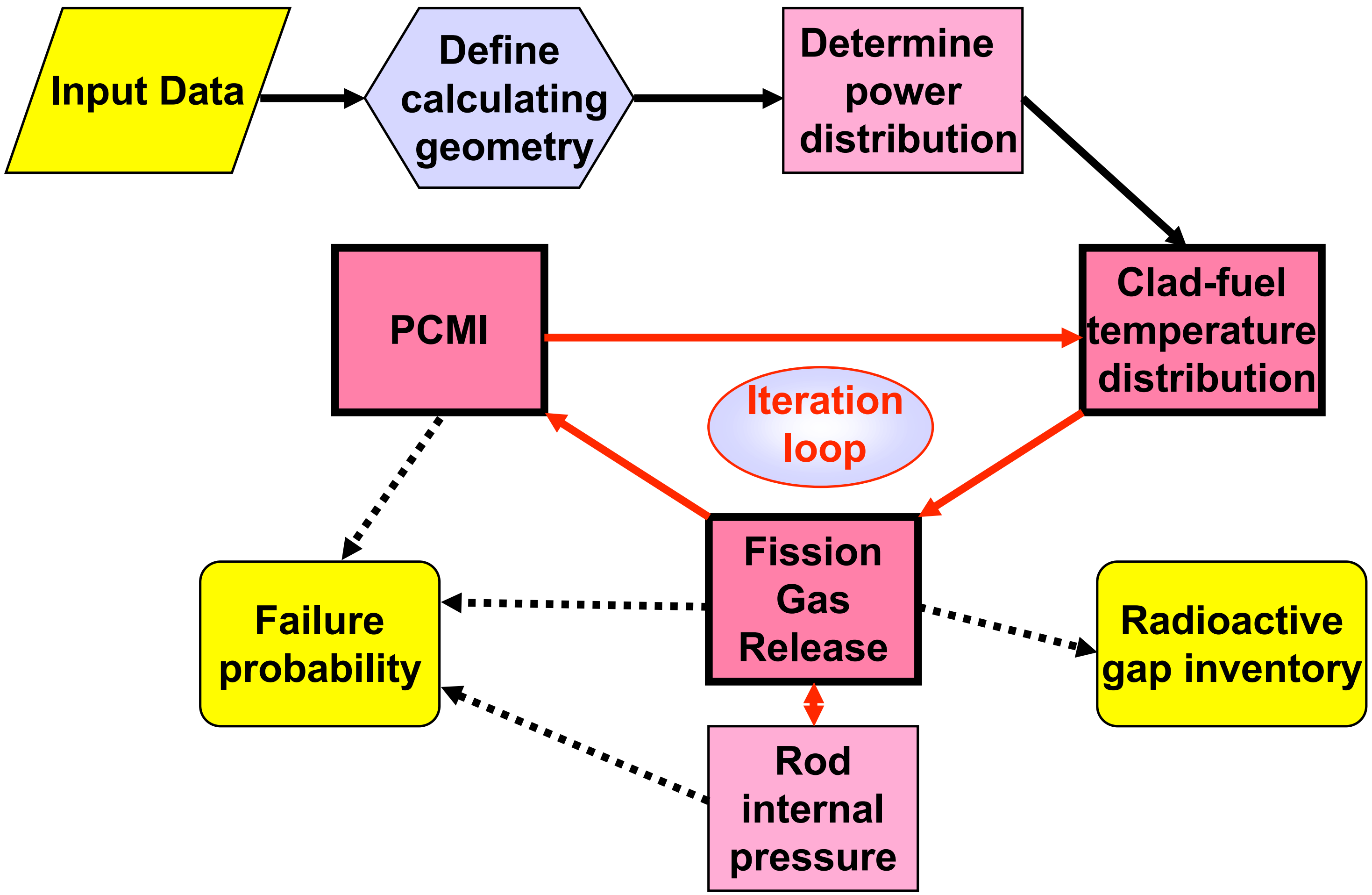
- Calculate the behaviour of a fuel rod during irradiation
  - steady state irradiation
  - transients
  - radiological source terms for accident analysis
- Applications include:
  - R & D purposes
  - design of fuel rods
  - design of new products and fuel cycles
  - support loading of fuel into a power reactor
    - compliance with safety criteria - safety case submissions

Ideally we want to predict ...

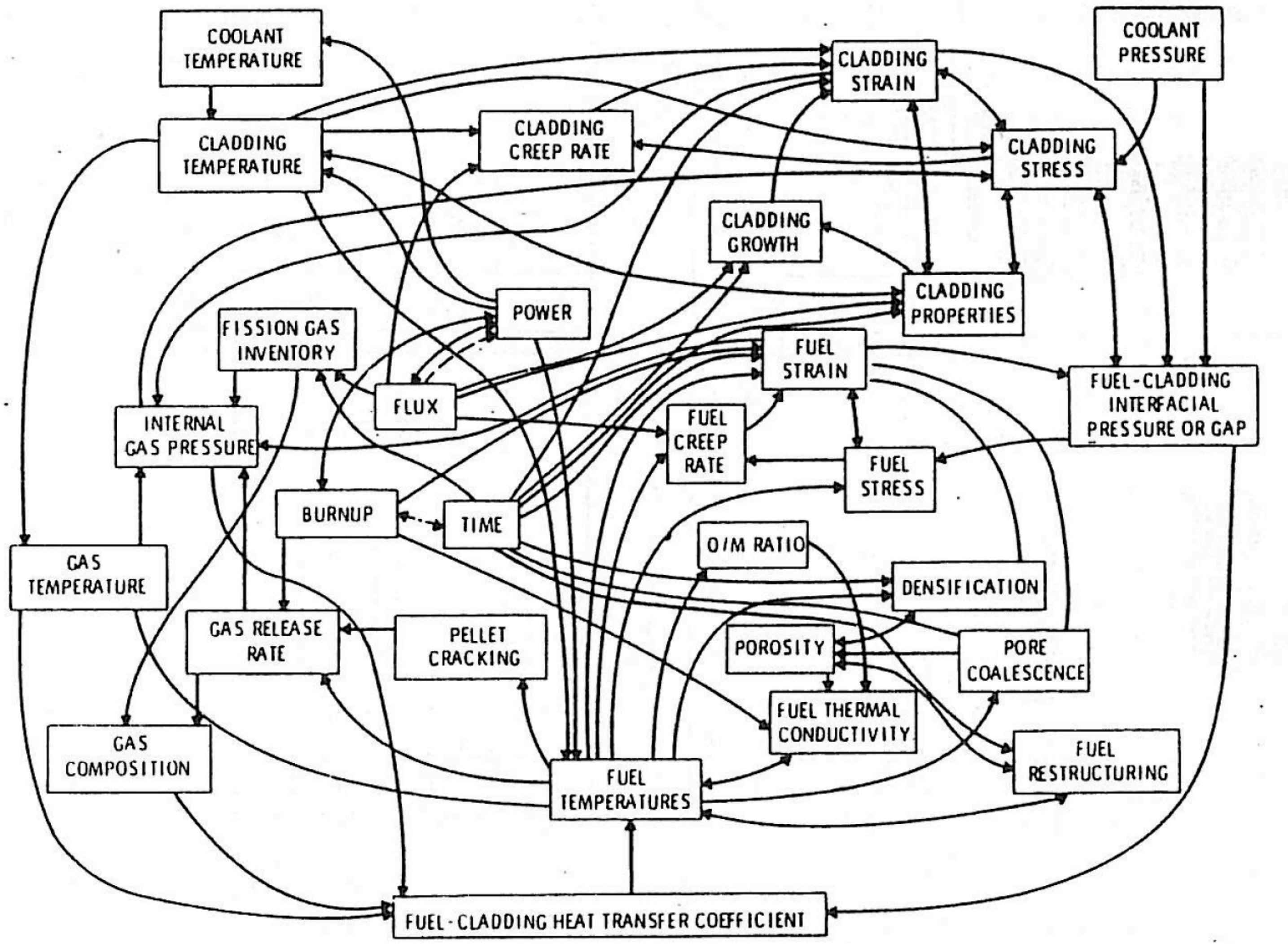


- oxide thickness
- temperature distribution
- stored heat
- clad diameter
- fuel diameter
- PCMI
- ridging?
- (crack distribution)
- porosity distribution
- grain size distribution
- FGR, ^{131}I inventory
- rod pressure
- did it fail?

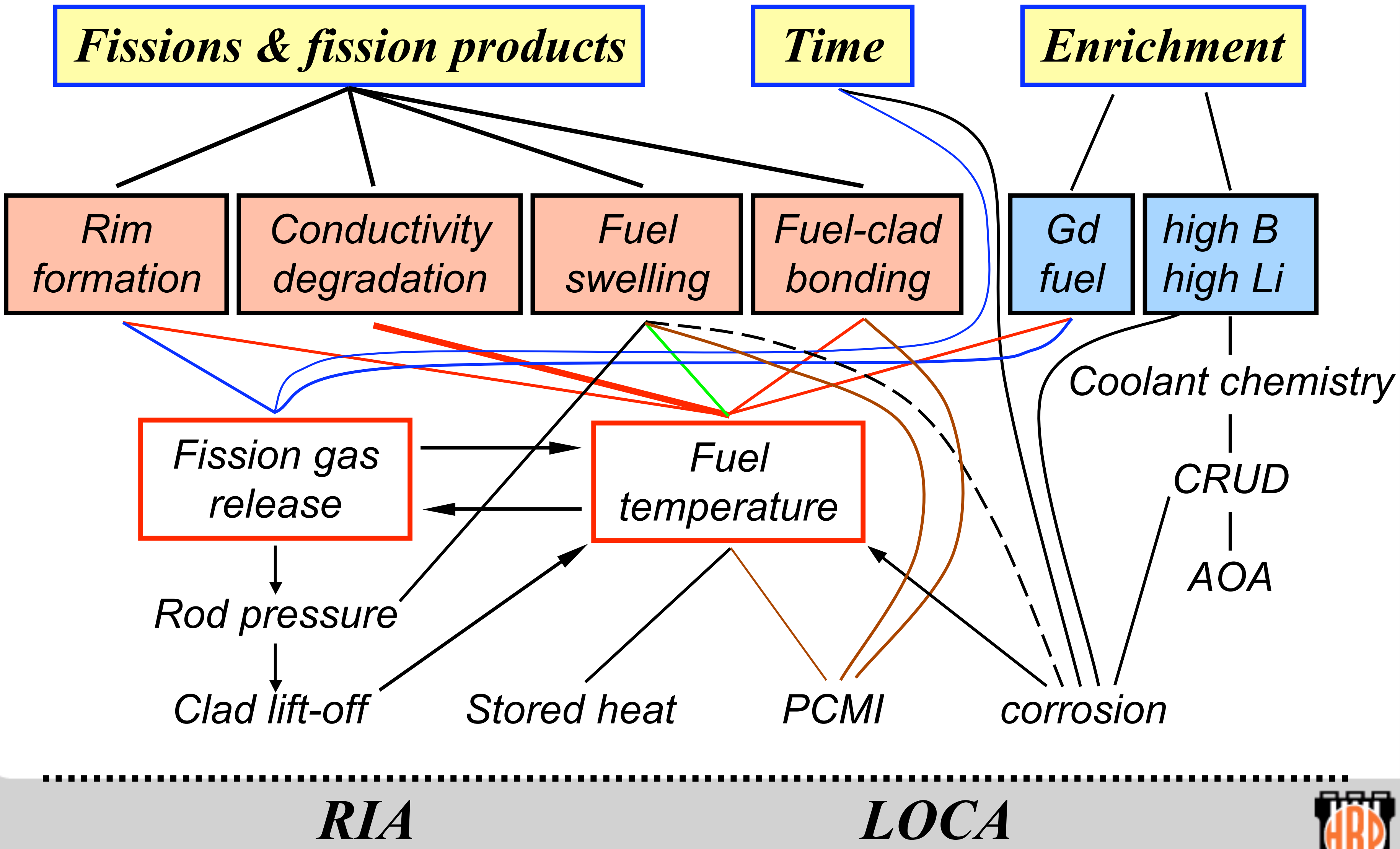
Typical code structure



... but it may be more complicated



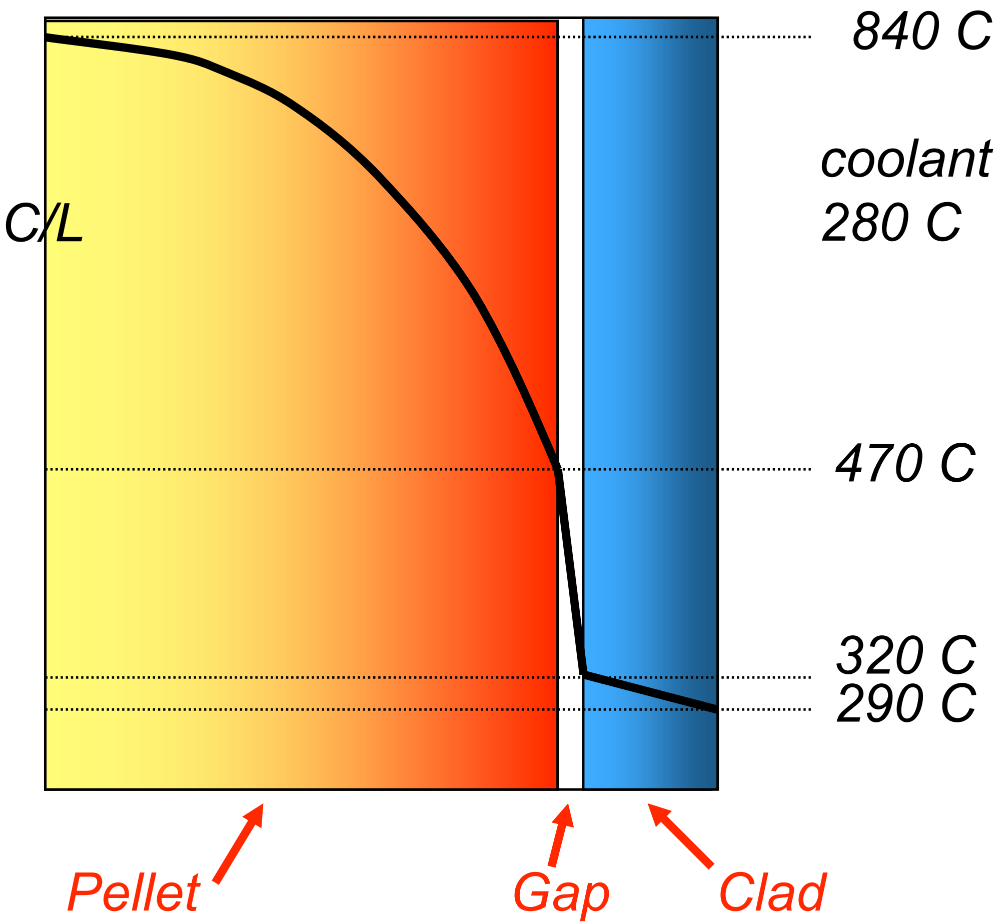
Fuel behaviour codes must address and untangle interactions that become more and more complex as fuel burnup increases



Fuel rod temperature distribution

- Many properties are exponentially dependent on temperature. Therefore accurate temperature estimates are important
- The fuel temperature is strongly linked to
  - stored energy that must be removed in LOCA
  - thermal expansion of the fuel pellet as strong contribution to pellet-clad mechanical interaction and rod failure
  - fission gas release and thus rod pressure
- The steady state temperature distribution can be calculated from outside to inside, starting from the fixed coolant temperature, without knowledge of the conditions inside.

Typical temperature distribution @ 20 kW/m



Heat flow resistances

- coolant – cladding
- oxide/crud layer
- cladding wall
- inner oxidation / bonding layer
- fuel – cladding gap
  - numerous influences (see ”spaghetti” graph)
- high burnup porous rim
- fuel
  - conductivity
  - porosity
  - cracks

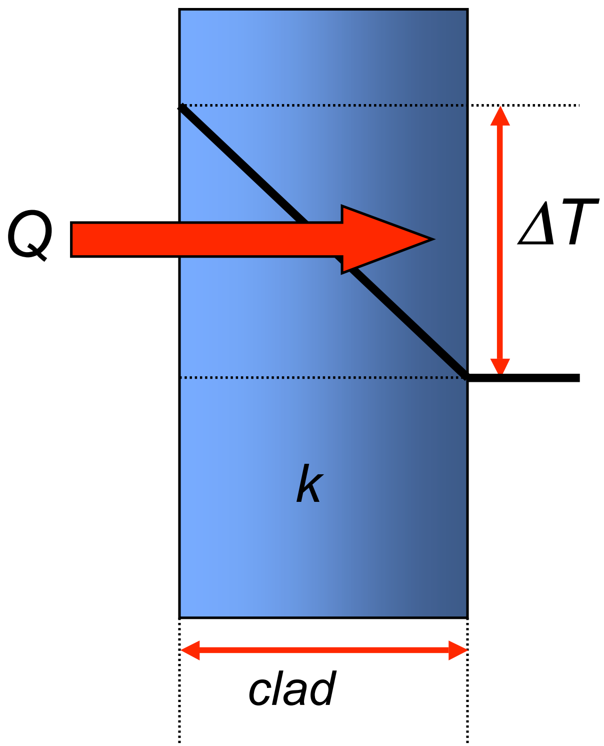
Fuel rod temperature calculation
(coolant – clad heat transfer)

- **PWR conditions:** Dittus - Boelter correlation
  $h = 0.023 * k/D_E * Re^{0.8} * Pr^{0.4}$
  k = water conductivity, D_E = equivalent diameter,
  Re = Reynolds number, Nu = Nusselt number.
- **BWR conditions:** Jens - Lottes correlation
  $T_{wall} – T_{sat} = 0.79 * \exp(-p/62) * (q'')^{0.25}$
  p = pressure (bar); q'' = heat flux, W/m^2
- $\Delta T_C = LHR/(\pi D \cdot h)$
  - typical ΔT_C at 250 W/cm = 25 K for PWR; 8 K for BWR

Fuel rod temperature calculation
(crud and oxide layer)

- Outer oxide layer
  - $\Delta T_{OX} = LHR / (\pi D \cdot k_{OX}/w_{OX})$
  - $k_{OX} = 0.015 \pm 0.005$ W/cmK;
    w_{OX} = 50-100µm for PWR fuel at high burn-up
    (a factor of ~3 lower for BWR fuel).
  - ΔT_{OX}= 20-80°C for LHR=250 W/cm in PWR
- Crud layer
  - constitutes a heat transfer barrier.
  - the crud thickness is normally moderate (some tens of µm at most)
  - conductivity is comparable to oxide conductivity.

Fuel rod temperature calculation
(temperature increase in the cladding)



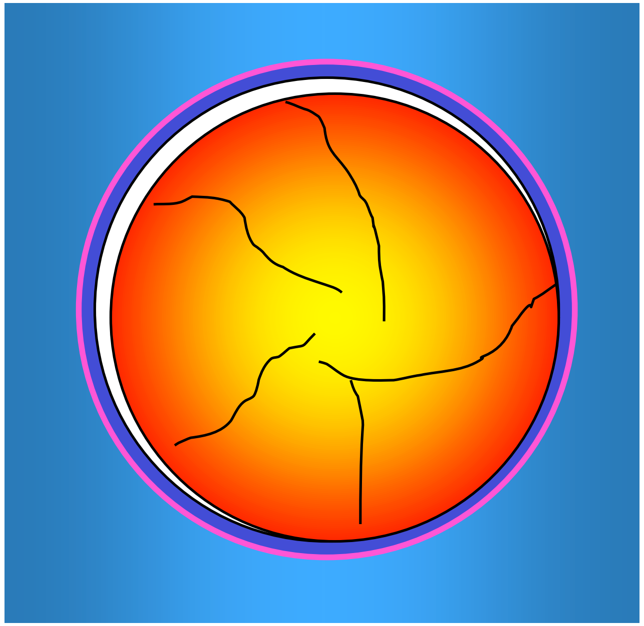
- *$\Delta T = 1/k*q'/2\pi*\ln(R_o/R_i)$*
  - *k = conductivity (W/mK)*
  - *q' = linear heat rating (W/m)*
  - *R_o, R_i = outer, inner clad radius (m)*
- *for typical wall thickness 0.6 - 0.9 mm, the problem can also be approximated in 1 dimension*
- *k ~ 20 W/m/K (linear function of T)*

Example: *ΔT for 0.6 mm thick clad of OD 10 mm at 20 kW/m?*

ΔT ~ 19 K

Fuel rod temperature calculation
(temperature step in the pellet-cladding gap)

- 3 conduction routes:
  - by radiation
  - through areas of contact
  - through the gas gap
- the pellet is usually eccentrically located in the cladding tube
- treatment in one dimension with effective heat transfer coefficient
- $h_{eff} = h_{rad} + f*h_{cont} + (1- f)*h_{gas}$
- proper averaging (f) of contact and gas conductance is important for good results
- model details depend on numerous properties and results from other part of a fuel behaviour modelling code



Temperature step in the pellet – clad gap

- radiative heat transfer -

Stefan-Boltzmann constant

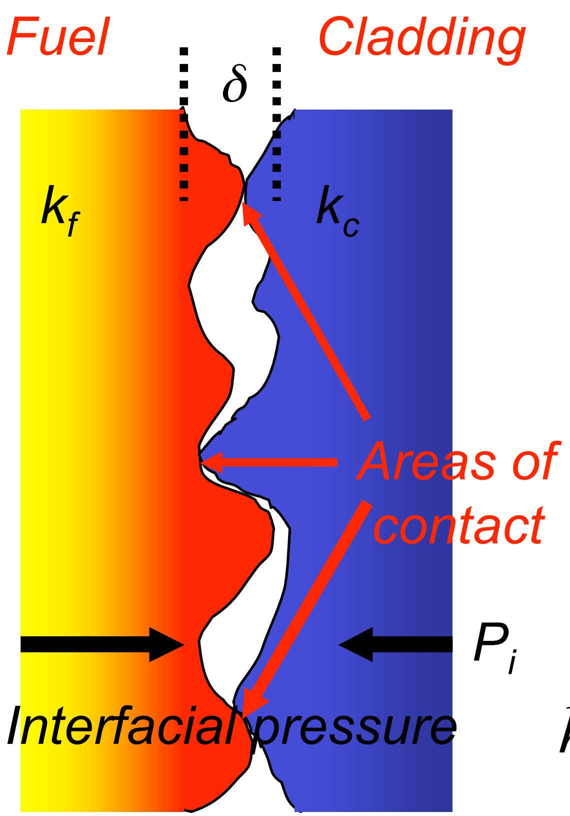
Mid gap temperature (K)

$$h_{radiation} = \frac{4 \cdot \sigma \cdot T^3}{(1/\varepsilon_f) + (1/\varepsilon_c) - 1}$$

Fuel & clad emissivities

- *Small contribution under normal operation*
- *no dependence on gap size since ratio of inner and outer radii is practically 1 (small gap)*

Temperature step in the pellet – clad gap
- contact conductance -



Occurs even for open gaps due to pellet eccentricity

Several theories mostly based on circles of contact whose number or area increases with interfacial pressure

A typical equation has the form:

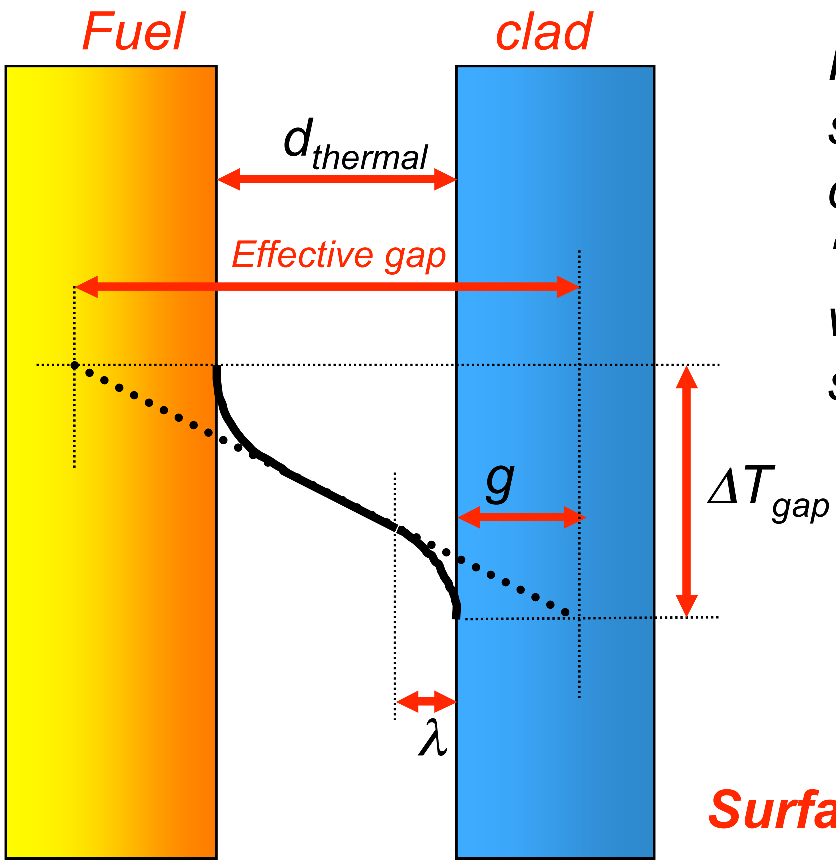
1 - 0.7

$$h_{contact} = Const.\left(\frac{2k_f k_c}{k_f + k_c}\right)^{\beta} \cdot \frac{P_i}{\delta^{1/2} \cdot H}$$

Fitted to data

Meyer hardness

Temperature step in the pellet – clad gap
- gas conductance through the gap-



Imperfect heat transport across solid-gas interface leads to the concept of a:
"Temperature Jump Distance" (g)
which effectively increases the gap size:

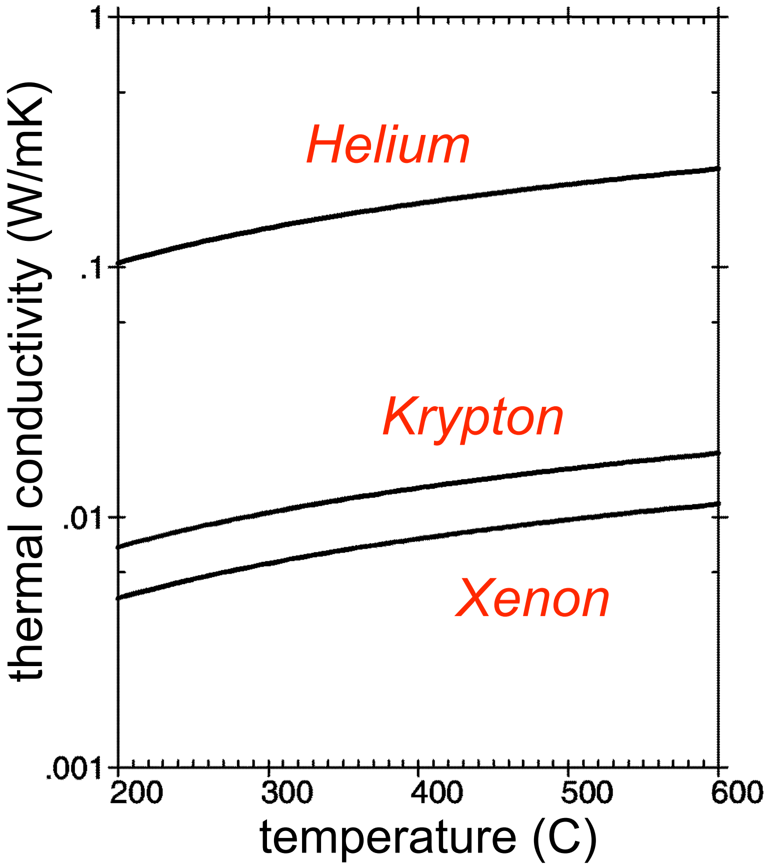
$$h_{gas} = \frac{k_{gas}}{\delta + d_{thermal} + 2g}$$

Surface roughness (δ)

Temperature jump distance ($2g$)

Gas conductivity

Gases are not good heat conductors (good insulation)



$$k_{gas} = A \cdot 10^{-4} \cdot T^{0.79}$$

k_{gas} (W/m/C) and T(K)

A =	*15.8*	*He*
	1.15	*Kr*
	0.72	*Xe*

Note: independent of pressure

For a gas mixture: xHe & (1-x)Xe

$$k_{mix} = (k_{He})^{x} \cdot (k_{Xe})^{(1-x)}$$

(von Ubisch rule, more complicated formulations exist)

Temperature jump distance

The Halden FTEMP code uses this empirical expression:

$$2g(\mu m) = \frac{(10 - 9 * x_{Xe})}{P}$$

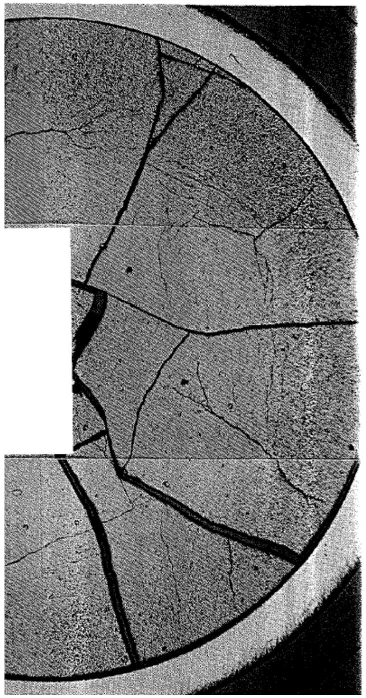
x_{Xe} = *fraction of Xe in He*
P = *gas pressure (ata)*

This equates to $2g_0$ values at STP of:

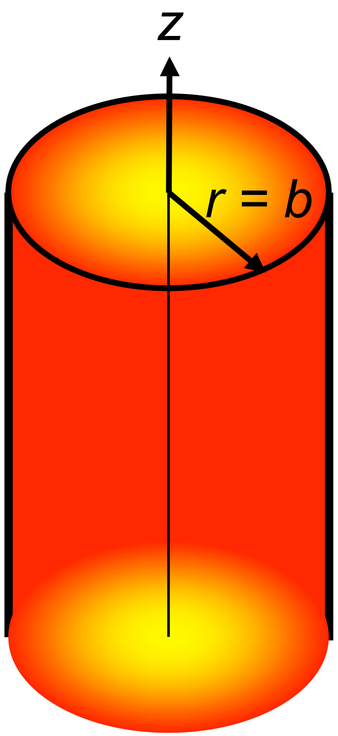
~6 .6 μm	He
~0.66 μm	Xe

... and the gap?

- The phenomena and properties mentioned before (with complexity of description ranging from constants and empirical equations to formulations based on first principles) are important parts of gap heat transfer modelling. However
- the most important quantity is the **pellet-clad gap**. It depends on
  - differential thermal expansion of fuel and cladding
  - fuel cracking and relocation,
  - distribution of open and closed gap
  - fuel densification and swelling
  - clad creep-down
  - interfacial pressure (calculated by other models)
- Many of these phenomena
  - are stochastic and cannot be calculated exactly
  - depend in complicated ways on other phenomena
- **The calculation of the heat transfer between pellet and cladding remains a source of uncertainty**



Fuel rod temperature calculation
(temperature distribution in the fuel)



A_0 = *Heat production per unit volume*

Steady state radial heat flow in a cylinder

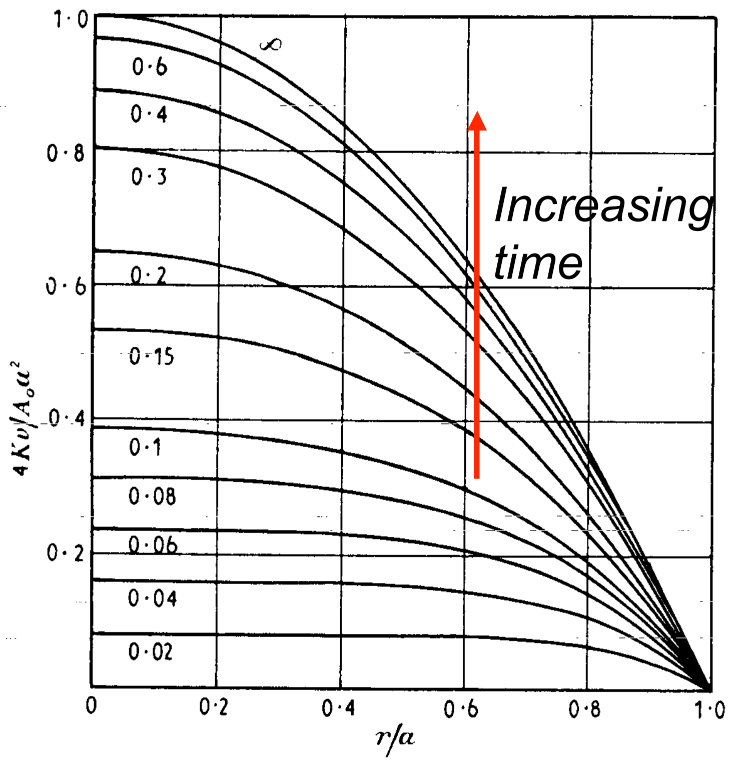
$$\frac{1}{r} \cdot \frac{d}{dr}\left(r \cdot \frac{dr}{dT}\right) + \frac{A_0}{k} = 0$$

Hollow cylinder a < r < b

$$T_c = T_s + \frac{A_0}{4k} \cdot \left(b^2 - a^2 \cdot \left(1 - 2\ln\left(b / a\right)\right)\right)$$

The principal temperature distribution is parabolic. Fuel conductivity k is space dependent, *k* = *k(T(r))*; also the heat production depends on location. For computational purposes, the fuel is therefore divided into rings, and the problem is solved with averaged properties per ring. Iterative solution because of the temperature dependence.

Fuel rod temperature calculation
(temperature distribution in the fuel)



Time dependent temperature distribution

Equation:

$$\frac{1}{r}\cdot\frac{d}{dr}\left(r\cdot\frac{dr}{dT}\right)+\frac{A_0}{k}=\frac{\rho\cdot Cp}{k}\cdot\frac{dT}{dt}=\frac{1}{K}\cdot\frac{dT}{dt}$$

diffusivity

Solution:

Bessel functions

$$T_r=\frac{A_0\cdot\left(a^2-r^2\right)}{4k}-\frac{2A_0}{ak}\sum_{n=1}^{\infty}e^{-K\alpha_n^2 t}\cdot\frac{J_0(r\alpha_n)}{\alpha_n^3\ J_1(a\alpha_n)}$$

Because of the space dependence of the heat generation and the thermal properties, the problem is usually solved numerically on the differential equation level.

... but we need some more details

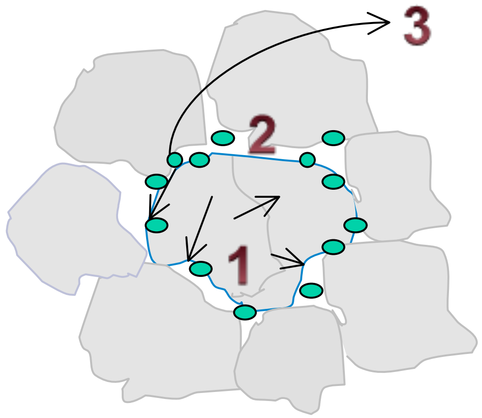
- Thermal conductivity of the fuel
  - temperature dependence
  - burnup dependence
  - influence of additives (e.g. Gd)
- Influence of porosity on conductivity
  - densification (removal of pores)
  - generation of new porosity by fission gas
- Influence of fuel cracking
- Radial power distribution (is not constant)
  - changes due to burnup and Pu generation (solution may be left to nuclear physics codes)

Each of these would require their own lecture

Fission gas release

- Fission products are responsible for
  - fuel swelling and PCMI (solid fission products)
  - stress corrosion cracking and failure (iodine)
  - pressure build-up in the fuel rod (xenon, krypton)
    - feedback on gap conductance and fuel temperature
    - rod overpressure and clad lift-off
    - driving force for ballooning during LOCA
  - pressure build-up in the fuel pores
    - fuel fragmentation and expulsion during RIA and LOCA
    - gaseous swelling and PCMI (failure)
- Rod pressure is limited by safety criteria and must therefore be calculated for the safety case

Fission gas release
- basic mechanisms -



- Fission gas atoms diffuse from within the fuel grain to the grain surface (temperature driven)
- The fission gas atoms accumulate at the grain surface in gas bubbles
- When the surface is saturated with bubbles, they interlink and the gas is released out of the fuel matrix
- FGR depends on temperature and burn-up (time)
- FGR is <1% for temperatures below ~1000-1200 ^{o}C and ~10-20% at ~1500 ^{o}C

Fission gas release

- phenomena involved -

1. Recoil
2. Knock-out & sputtering
3. Lattice diffusion
4. Trapping
5. Irradiation re-solution
6. Thermal re-solution
7. Densification
8. **Thermal diffusion**
9. Grain boundary diffusion
10. Grain boundary sweeping
11. Bubble migration
12. **Bubble interconnection**
13. Sublimation or vaporisation

Fission gas release
- basic thermal diffusion model -

- Fission gas release was observed very early on and explained by diffusion out of the fuel grains (Booth)
- Assumptions for (simple) model:
  - atomic diffusion in hypothetical sphere
  - grain boundary = perfect sink
  - gas at grain boundary immediately released (?)
  - constant conditions of T and F
  - Solution (Booth diffusion, release rate)

$$f_{irr}(t);\ 4\sqrt{\frac{Dt}{\pi R_{gr}^2}}-\frac{3}{2}\frac{Dt}{R_{gr}^2}$$

Diffusion coefficient

$$D = D_a + D_b + D_c$$

- Thermal coefficient (T>1400^{0}C)

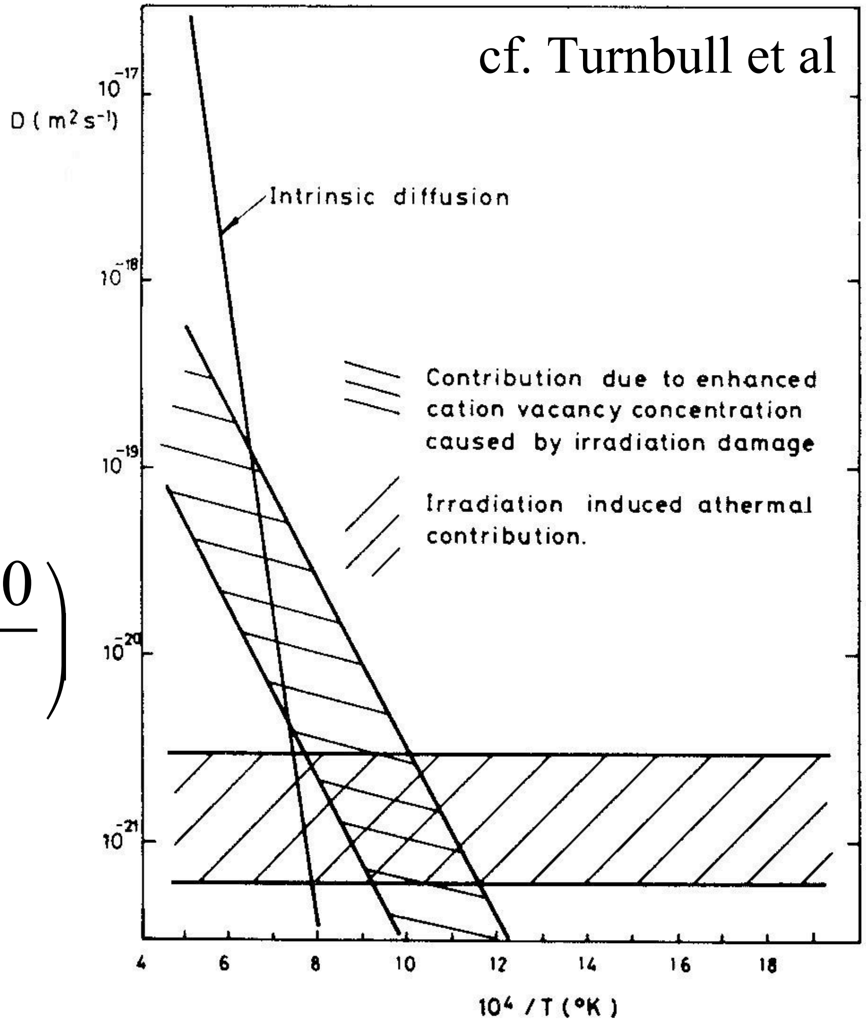
$$D_a = D_0 \exp\left(-\frac{\Delta H}{RT}\right)$$

- Intermediate

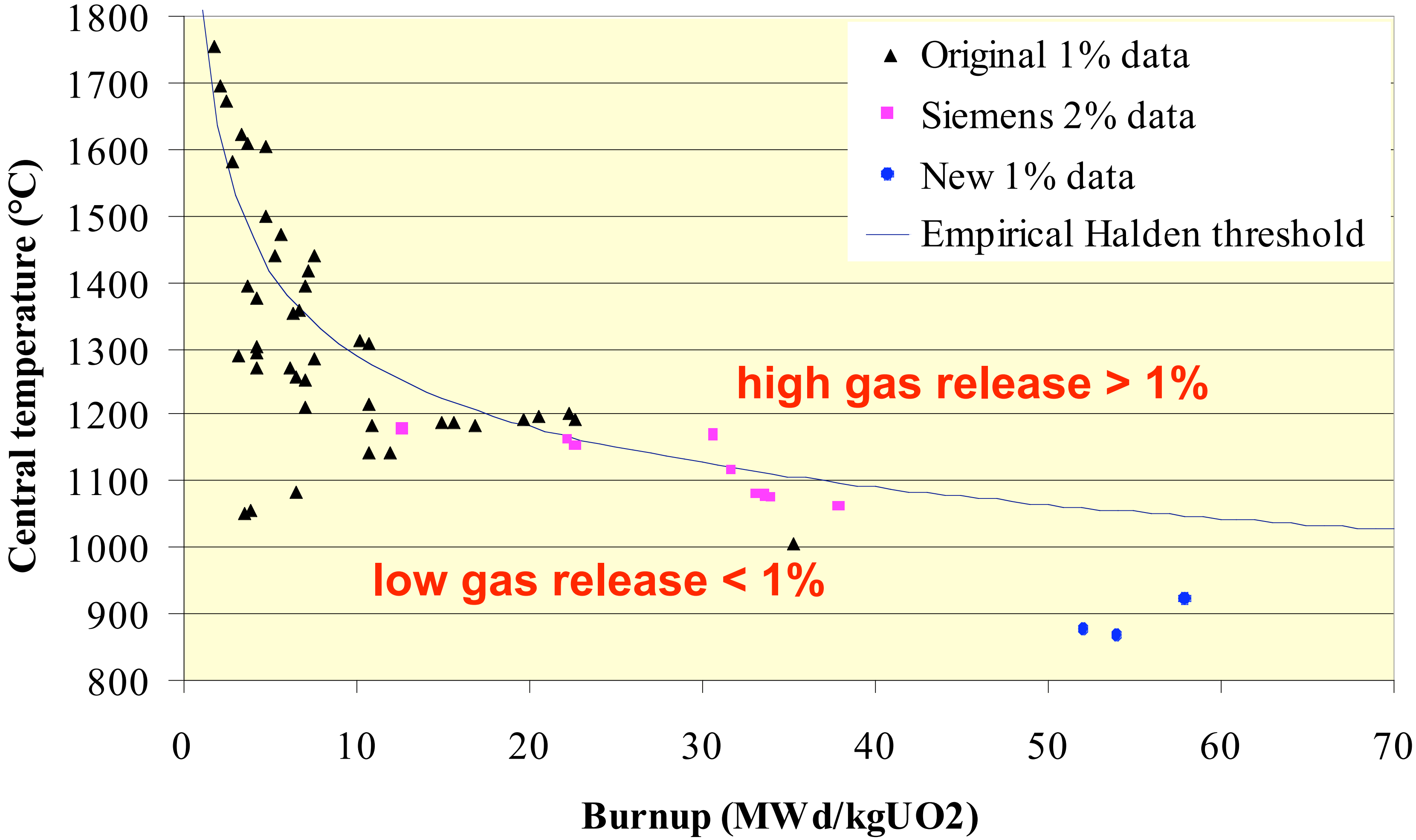
$$D_b = 6.64 \cdot 10^{-25} \sqrt{\dot{F}} \exp\left(-\frac{13800}{T}\right)$$

- Athermal coefficient (T<1000^{0}C

$$D_c = A \cdot \dot{F}$$

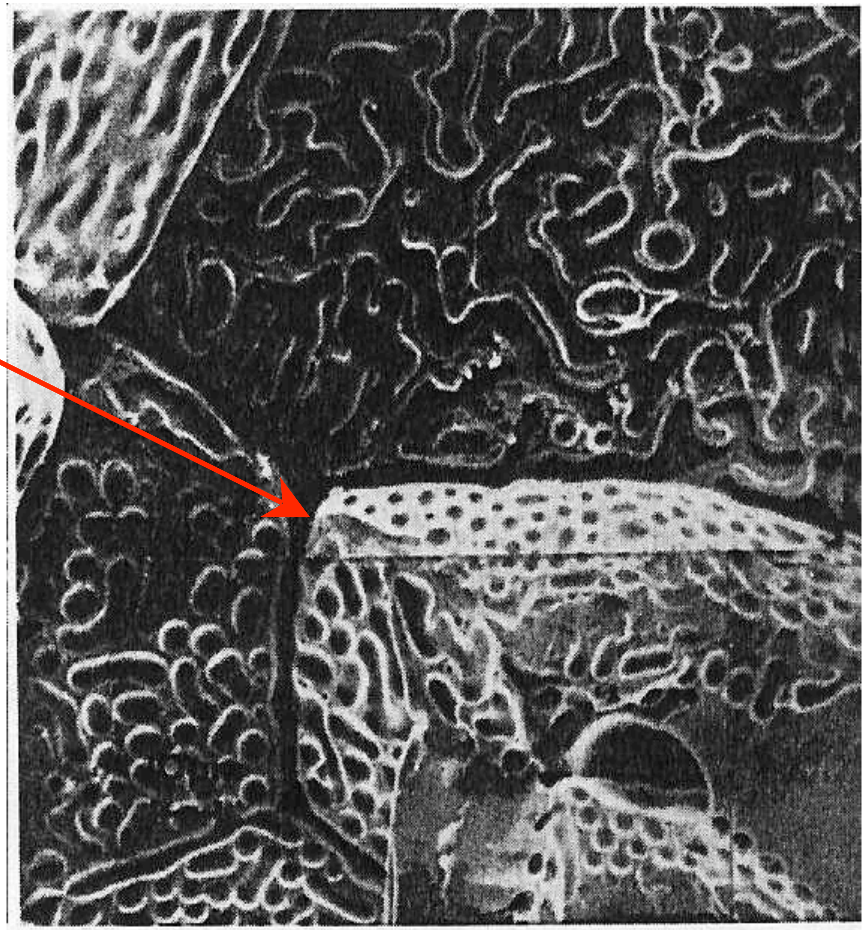


Observation: incubation threshold



Fission gas release
- Bubble interconnection -

- **Explains incubation** and onset of (stable) fission gas release during normal operation due to increase of open surface (*open tunnel network)*
- **Explains burst release** (micro-cracking) during abrupt power variations → requires precise knowledge of local stress

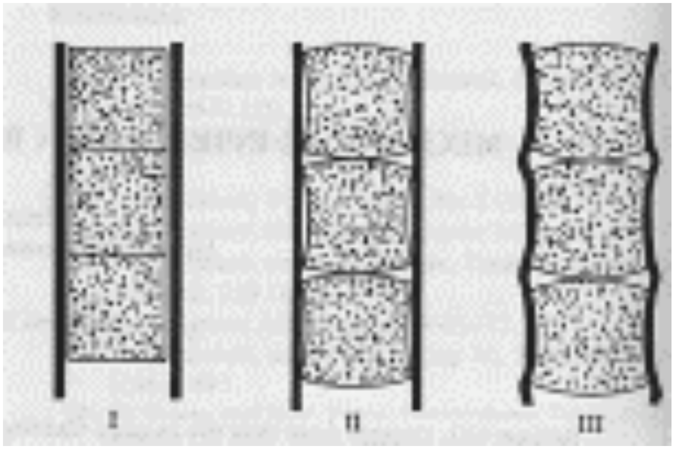


FGR models

- Large number of models
  - Improvements
    - numerical techniques
    - new mechanisms
  - Various applications: conditions, reactor types, …
- Large uncertainties
  - (mechanistic) model parameters
    - diffusion coefficient
    - resolution, ...
  - input parameters:
    - temperatures
    - hydrostatic stress, ...

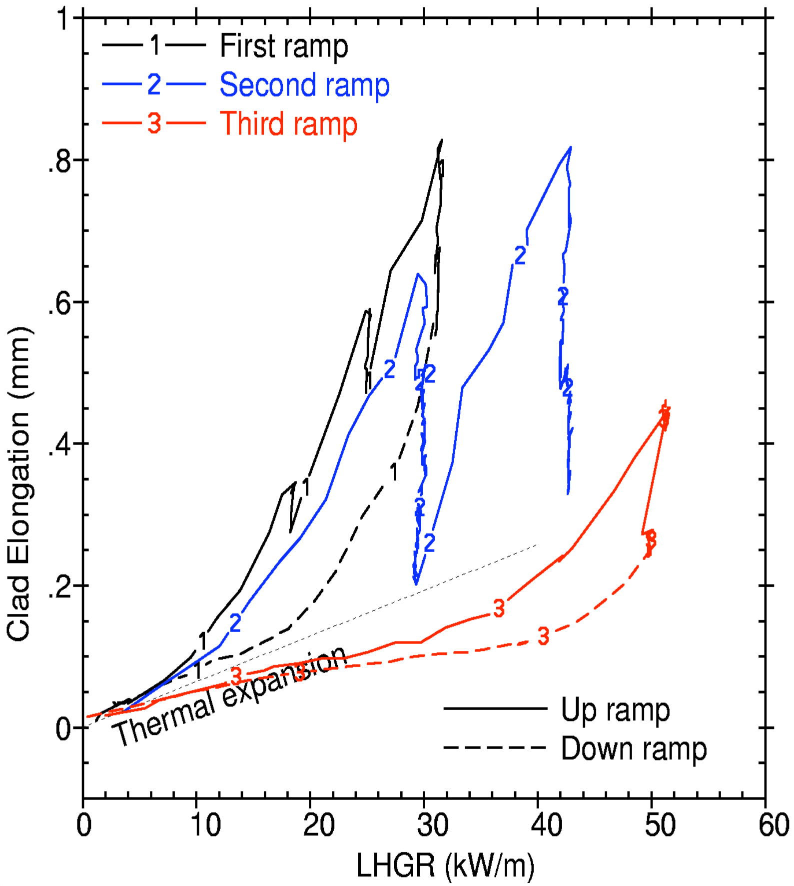
Dimensional changes and mechanical loads

- Reversible
  - Elastic deformation
  - Thermal expansion
- Partly reversible
  - Cracking
  - Fragment relocation
- Permanent
  - Plastic deformation
  - Creep
  - Fission product swelling
  - Densification



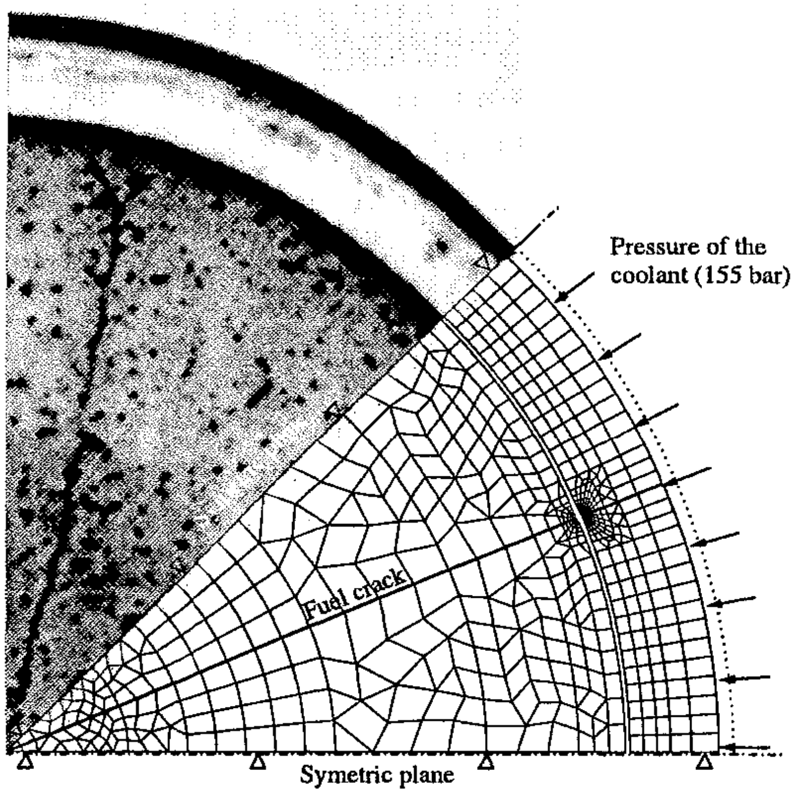
Thermal expansion of the pellet in a temperature gradient causes "ridging" at the pellet-pellet interfaces (also called wheat-sheafing, hour glassing)

PCMI and Fuel Cladding Length Change



- Fuel-clad gap closes due to clad creep-down and fuel swelling
- Power ramps induce fuel swelling and promote gap closure and thus PCMI
- PCMI has diametral and axial components
- Plotting cladding elongation (axial) as a function of rod power is typical for interpreting what is occurring
  - Onset of interaction (power at which PCMI first occurs) as function of BU
  - Cladding relaxation during power hold (slippage or fuel creep)
  - Degree of contact (soft or strong)

Modelling the observations



Axial and diametral deformation show similar trends

A “rigorous” treatment requires a 3D FEM description and is restricted to a few pellets.

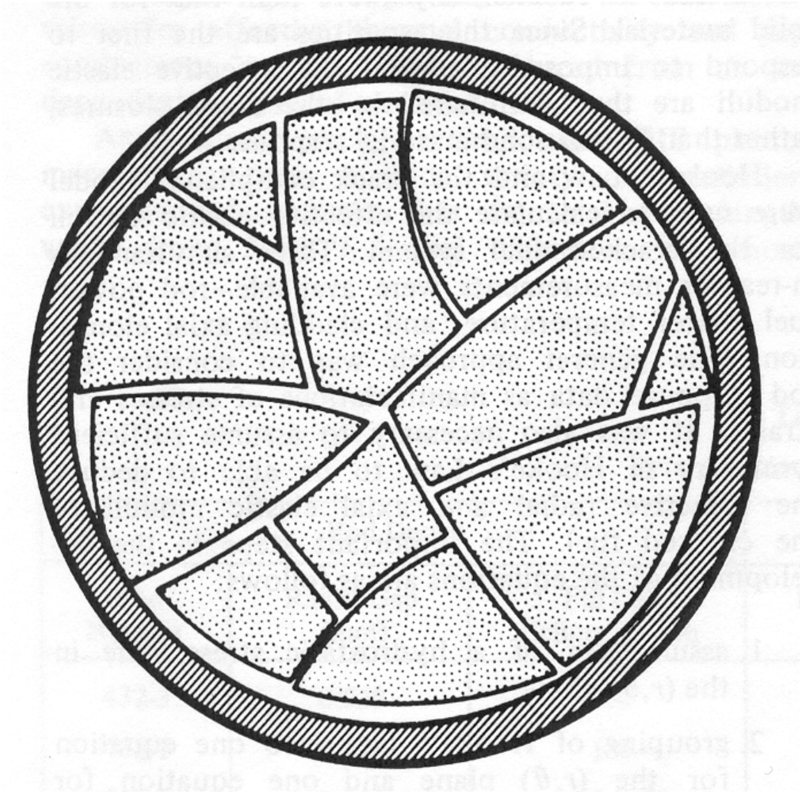
Treatment in fuel behaviour modelling

- 1 ½ D codes
  - axi-symmetric 1D model (radial dependence only) does not allow direct calculation of ridge formation
  - axial length (z direction) is divided into nodes
  - axial coupling of nodes
- 2D – 3D codes
  - more rigorous description of the geometry, but ...
  - restricted to a few pellets (2D: axi-symmetric r-z)
  - special coupling elements
- Codes must consider relative movement between pellet and cladding: no contact, frictional sliding, sticking
- Many 1 ½ D codes reduce the problem to sticking and thus avoid the complications of axial coupling (a reasonable approximation valid for many situations, but not always)

Modelling Considerations for 1D

- 1D (1½D) is a compromise with approximations
- To calculate the slope of a pile of sand (or coal or Norwegian boulders or …) with some accuracy, we do not have to calculate and determine the interaction between all grains.
- Despite the differences, a single model describes the situation.
- Can cracked fuel pellets within the cladding be treated like a pile of sand?

Modelling Considerations for 1D



- Experimental observations are difficult to reconcile with predictions of models assuming a concentric arrangement of fuel and cladding and a dividing gap
- Williford et al. proposed a crack compliance model where all surfaces interact through roughness contact. The formulation links surface pressure σ and crack width *d*:

$$\frac{1}{2} erf\left(\frac{d}{R\sqrt{2}}\right) = \frac{\sigma}{\sigma + H}$$

- The model allows a unified treatment of thermal and mechanical behaviour suitable for the high burnup situation with bonded fuel

Origin and characteristics of codes (Fumex)

Code	Organization Country	Based on	Use	Special feature
BACO	CNEA Argentina	BACO	PHWR	UO2 & MOX
ELESIM	AECL Canada	ELESIM	CANDU	ANS5.4 fission product release
EIMUS	CRIEPI Japan	FEMAXI - 3	Evaluation BWR PWR HBWR	
ENIGMA	BE, BNFL, UK		PWR CAGR (BE) MOX (BNFL)	ridging, ^{131}I release
ENIGMA	VTT Finland	ENIGMA (UK)	WWER	E110 clad properties
FAIR	BARC India	Ni-1	PHWR AHWR	2D capability clad failure model UO2 & MOX
FRAPCON	USNRC		BWR, PWR	Licensing benchmark
FRAPCON (VO)	CIAE China	US version	design, operation and safety evaluation	clad failure model trans. code input
FUDA	BARC India		design & licensing	ridging clad failure model

Origin and characteristics of codes (Fumex)

Code	Organization Country	Based on	Use	Special feature
PIN-micro	REZ Czech Rep	GT-2 PIN	LWR WWER	
PIN-W	RezCzech Rep	PIN-micro	WWER licensing	
PROFESS	BARC India		PIE analysis	UO_2 & MOX
ROFEM 1B	INR Romania	FEMAXI-3	PHWR CANDU	
START-3	IIM Russia		fuel behaviour R&D	Fuel failure calc.
TRUST	NFD Japan		R&D Fuel design	
TRANSURANUS	ITU Germany	URANUS	Fuel behaviour R &D	MOX, UC, UN fast reactor, Monte Carlo
TRANSURANUS	PSI Switzerland	ITU version	Fuel behaviour R &D	
METEOR	CEA France	ITU code	Fuel behaviour R &D	
COPERNIC	FRAMATOME France	TRANSUR	BWR, PWR fuel design and licensing	
COMETHE-IV	Belgo Nucleaire, Belgium		BWR, PWR fuel design and licensing	
COSMOS	KAERI South Korea		Fuel performance analysis	
CYRANO-3	EDF France		PWR licens ing	
SIERRA	Siemens PC		BWR, PWR fuel design and licensing	

Origin and characteristics of codes (ANS Park City 2000)

Code	Organization Country	Based on	Use	Special feature
FRAPCON -2	USNRC	GAPCON THERMAL -2	BWR, PWR	Licensing benchmark
FRAPCON -3	USNRC	FRAPCON -2	BWR, PWR	Licensing benchmark
FRAPTRAN	USNRC	FRAPT -6	Transient analysis eg LOCA and RIA	Fast transient capability
SCANAIR	DRS/SEMAR France		Transient analysis eg LOCA and RIA	Fast transient capability
FRAS	Kurchatov Institute, Russia		Transient analysis eg RIA	Fast transient capability

The END