Trieste Workshop

Temperature Calculations

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Contents

- Overview of Codes and their Application
- Model Development and Code Validation
- Temperature Calculations
- Conclusions

Overview of Codes and their Application

Fuel Performance Codes are used to:

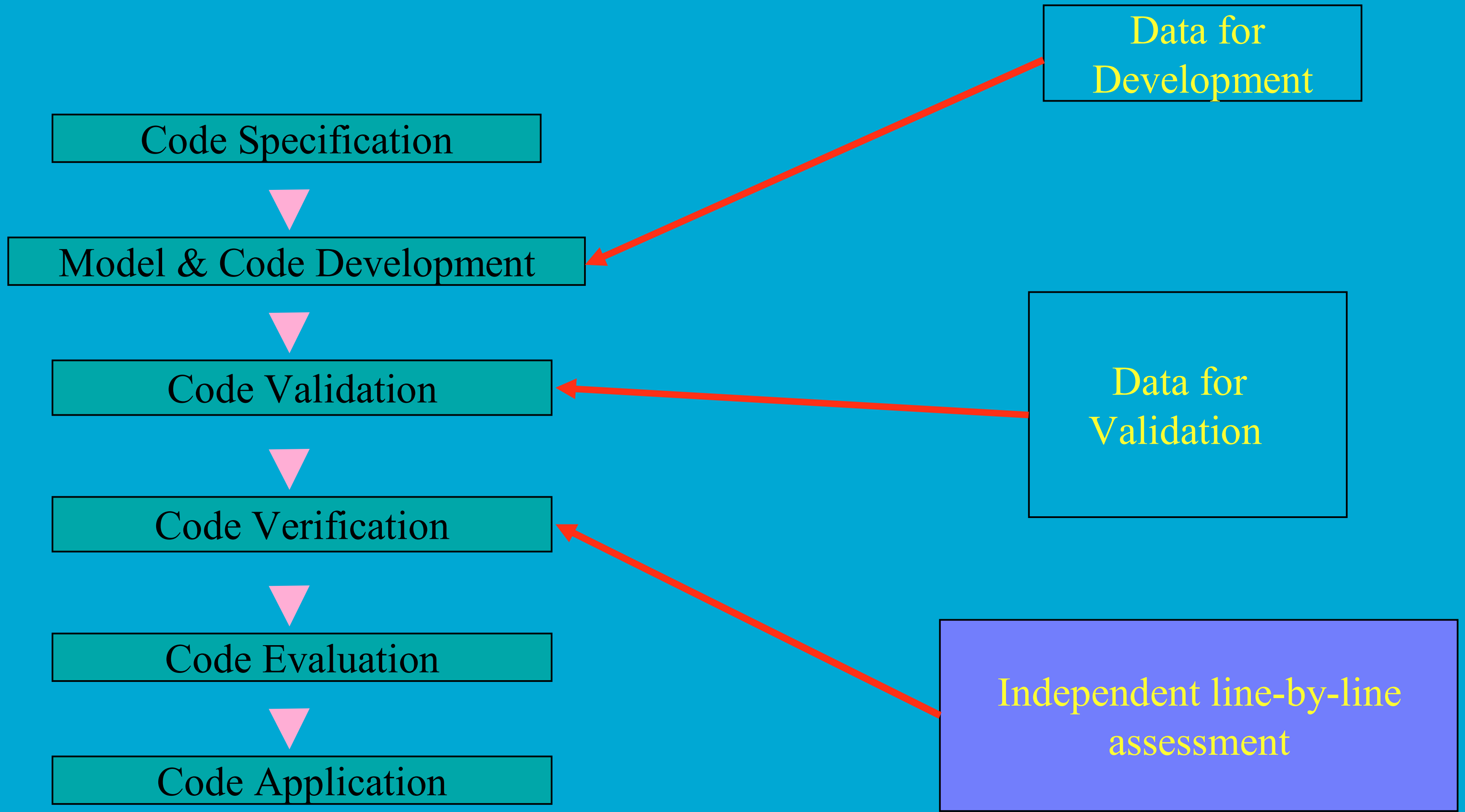
- calculate the behaviour of a fuel rod during irradiation
  - steady state irradiation
  - transient operation
  - calculation of radiological source terms for accident analysis

Applications include:

- for R & D purposes
- to design fuel rods
- to design new products and fuel cycles
- to support loading fuel into a power reactor
  - compliance - safety case submissions

Overview of Codes and their Application

Stages in code development



Code Specification

Model & Code Development

Code Validation

Code Verification

Code Evaluation

Code Application

Data for Development

Data for Validation

Independent line-by-line assessment

Overview of Codes and their Application

Input requirements:

- Reactor parameters,
    - PWR, BWR, WWER other……..
    - flux spectrum
    - coolant pressure & temperature distribution (PWR)
    - power versus time

- Fuel rod
    - assembly geometry, number of spacers etc...
    - total length, fissile stack length
    - plenum volume
    - fill gas composition and pressure

Overview of Codes and their Application

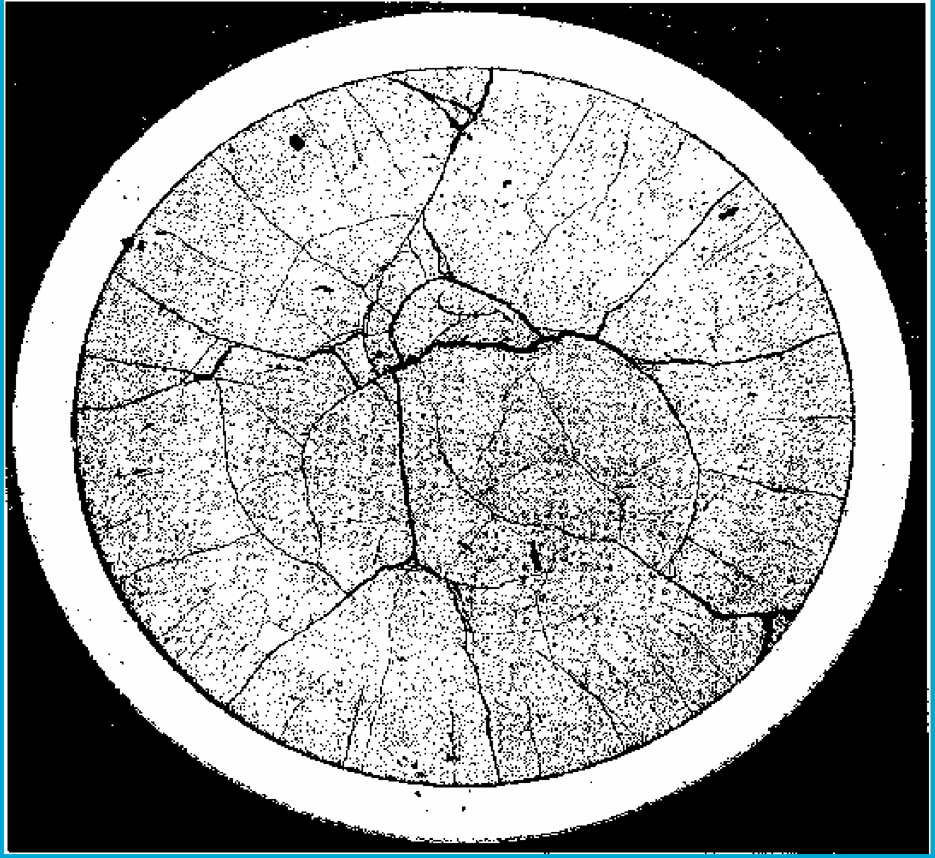
Input requirements (continued):

- Cladding
  - composition, Zr-2, Zr-4, E110 etc…….
  - external and internal diameters
  - presence of liners etc.
  - mechanical properties

- Fuel pellet
  - external and internal diameters
  - length, end geometry, dimple dimensions etc…….
  - enrichment, isotopic composition, ^{235}U, ^{241}Pu etc…….
    - Chemical composition, additives, stoichiometry…….
  - density, re-sintering test data
    - pore size distribution
  - grain size

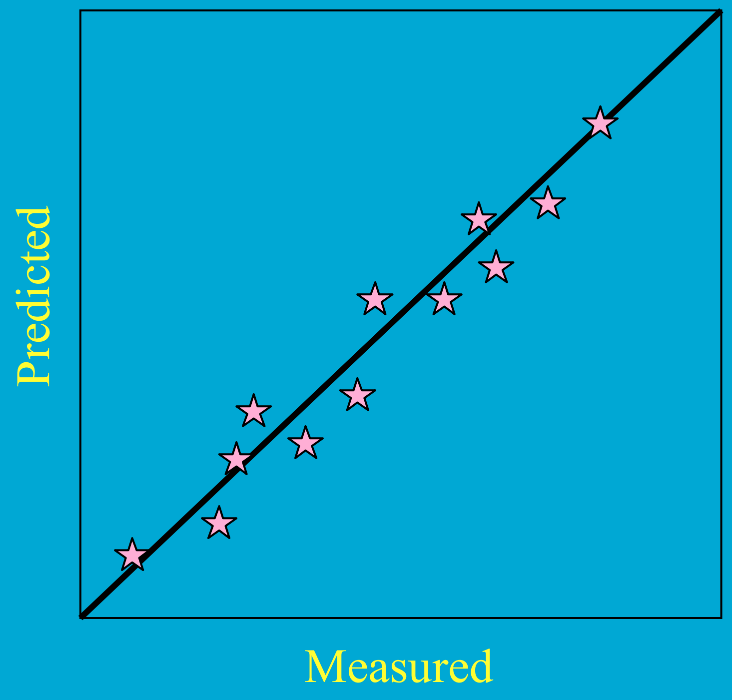
Overview of Codes and their Application

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?

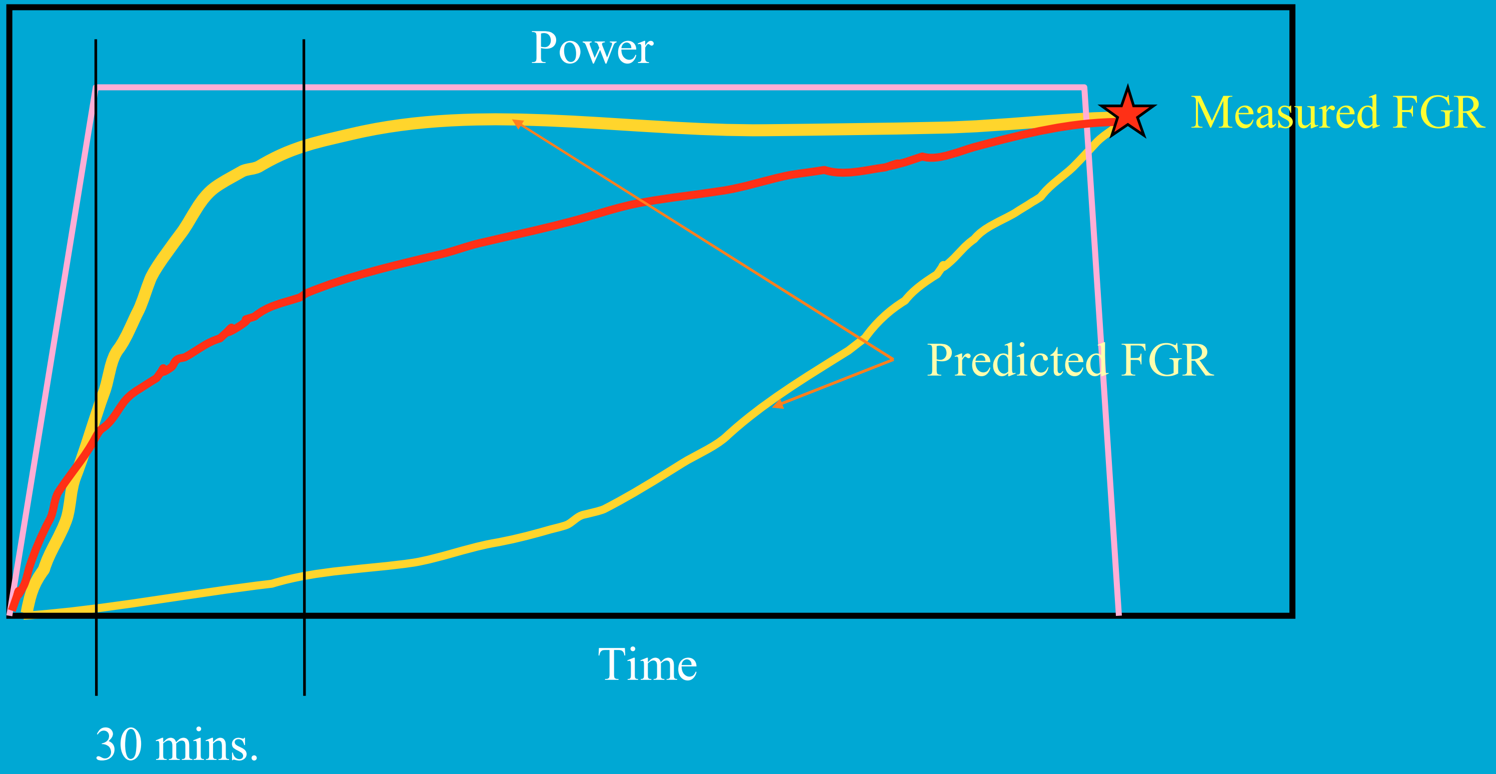
“Fitness for Purpose” judged through Code Validation



- Global P/M plots not adequate to demonstrate validation
- Need validation to demonstrate that models correctly reflect variation of parameters on predictions
- Database must provide adequate coverage of separate effects for *both* model development *and* validation

Model Development and Code Validation

Transient FGR



Evaluation

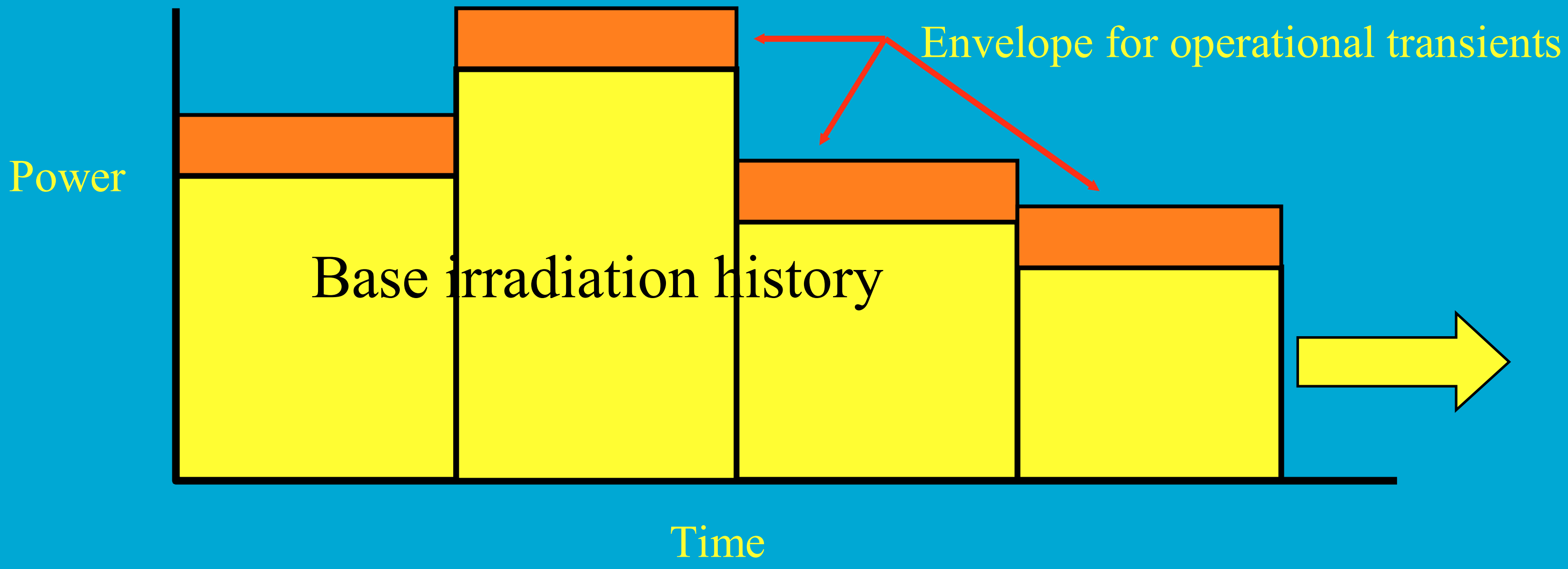
Evaluation of a code

- Simplified power histories to demonstrate that code behaves as expected, code is stable and insensitive to time step duration; there are no ‘cliff edges’ when extrapolating outside database
- Notional idealized power histories for safety cases demonstrates that predictions are within acceptable limits

Application of code

- After validation, for all applications, code should be run as a **‘Black Box’** with no changes made between runs

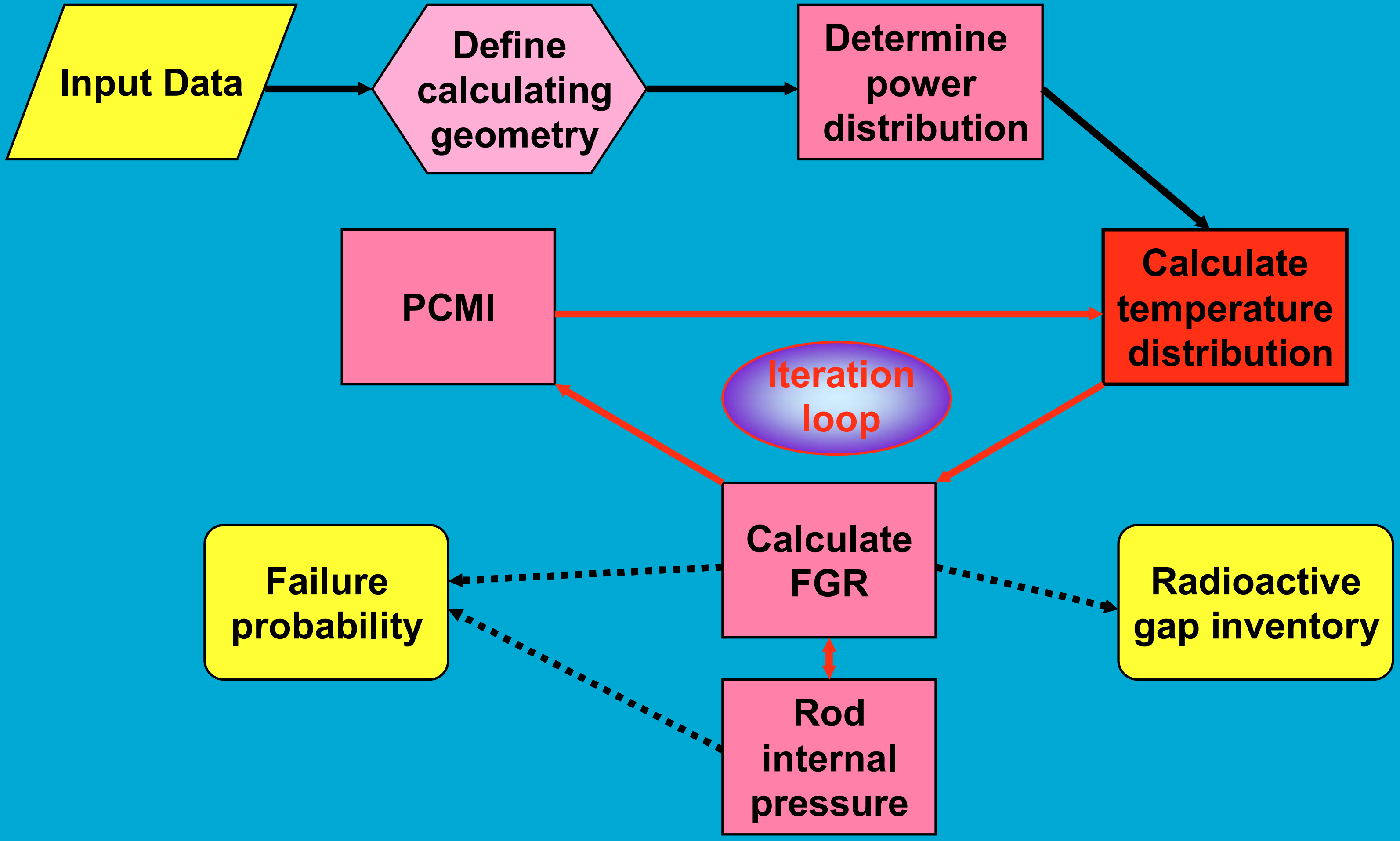
Application of code to fuel loading



Usual to adopt

- best estimate models with quantified modelling uncertainties
  e.g., FGR x / 2
- pessimistic rod & fuel parameters
- pessimistic irradiation history

Typical code structure



Input Data

Define calculating geometry

Determine power distribution

Calculate temperature distribution

PCMI

Iteration loop

Calculate FGR

Failure probability

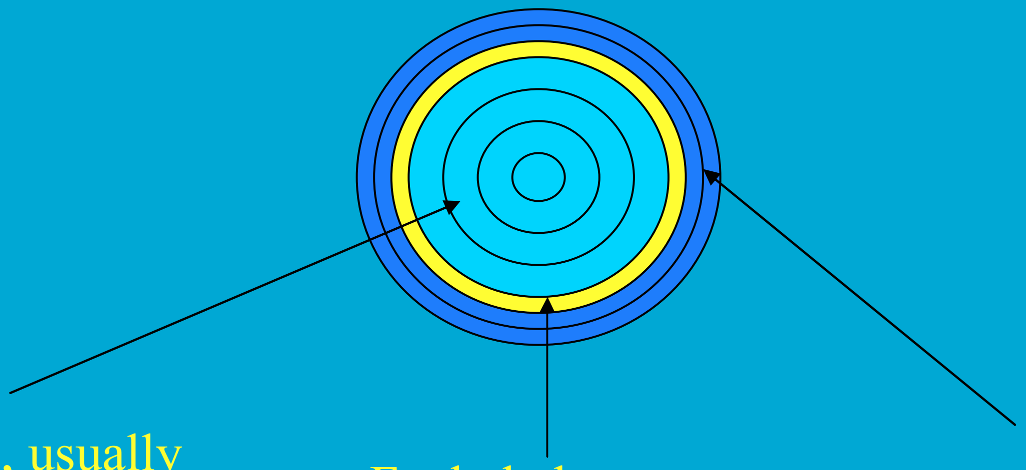
Radioactive gap inventory

Rod internal pressure

Radial and Axial calculations

The temperature is calculated in concentric rings using iterative approaches. The material properties will vary in each zone, as they are generally temperature dependent.

The local heat generation will depend on local power, which will increase at the pellet rim as burnup proceeds.



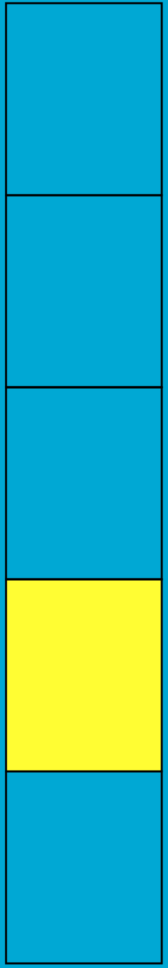
Fuel zones, usually
of equal volume

Fuel clad gap

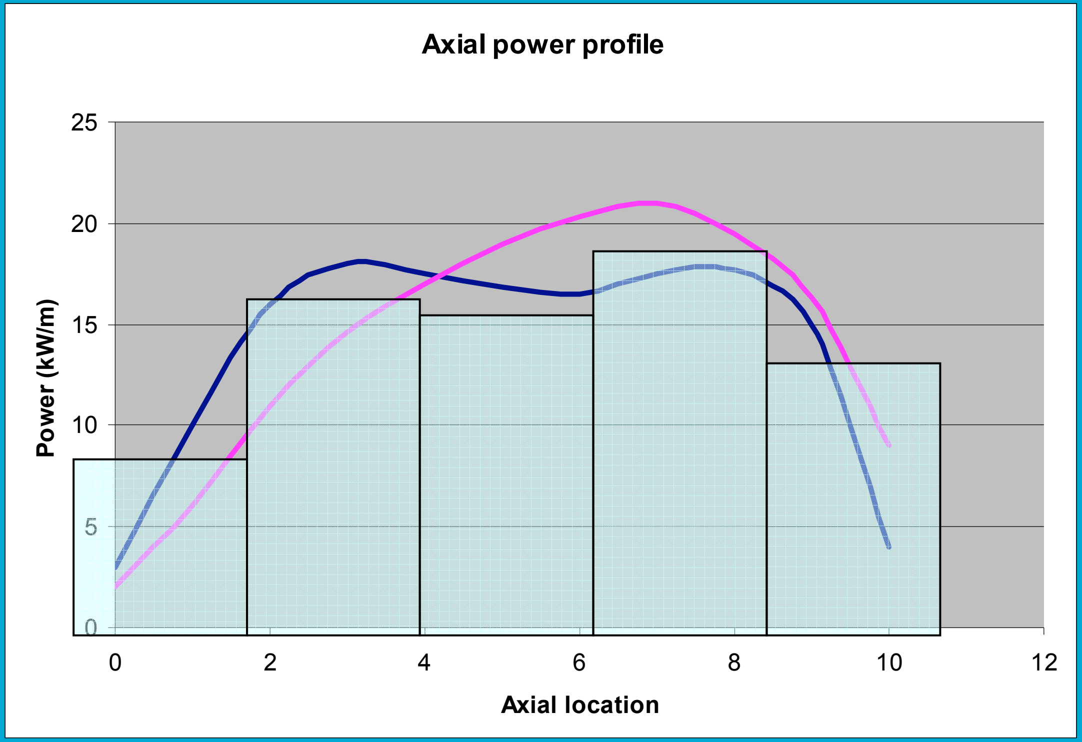
Cladding zones

Radial and Axial calculations

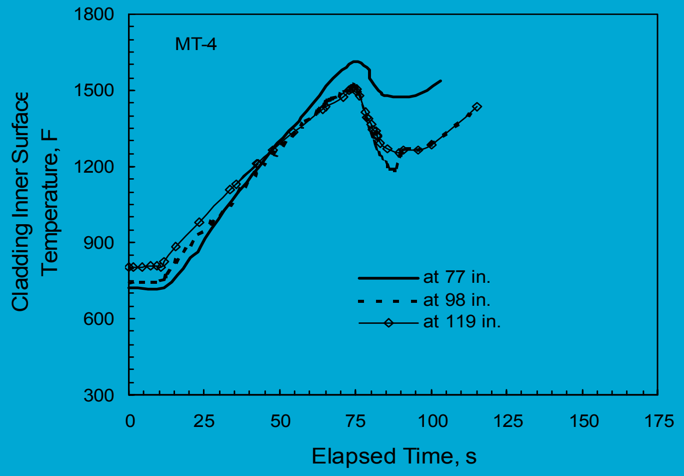
Axial power distribution

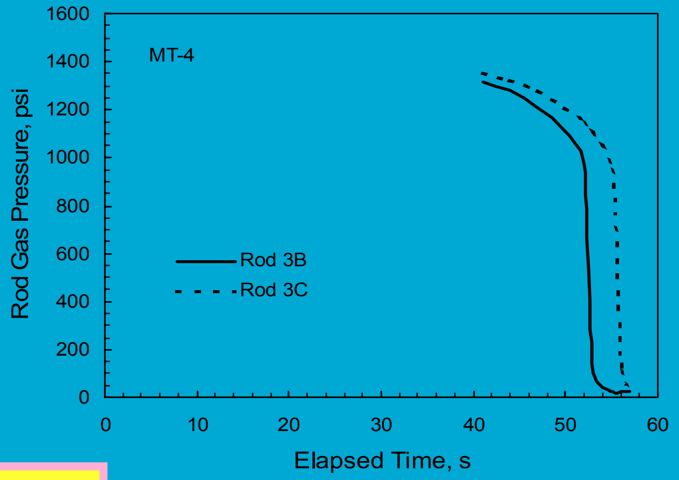


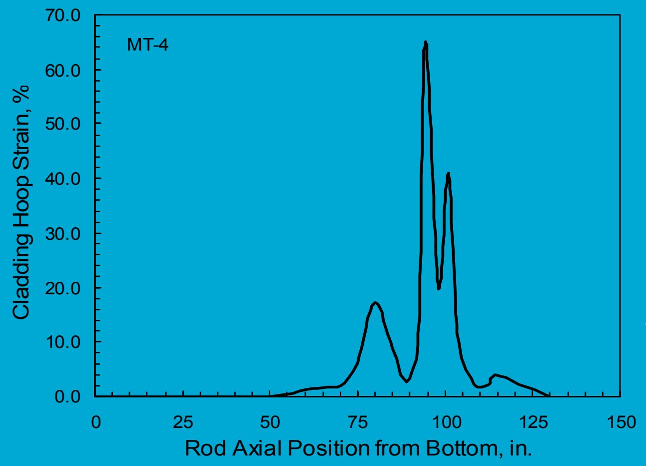
Axial power profiles vary during irradiation



Experiments: LOCA, NRU tests MT-4







Clad Temperature v time

Internal pressure v time

Resulting clad plastic strain

Initiating Events requiring calculation of fuel response

- Increase in heat removal
- Decrease in heat removal
- Reactivity and power distribution anomalies
- Increase in reactor coolant inventory
- Decrease in reactor coolant inventory
- Radioactive release from subsystems or components
- Fuel handling accidents
- Anticipated transients without scram (ATWS)

Initiating Events requiring calculation of fuel response

Categorization of transients

- Anticipated Transients
  - probability >10^{-2}/year
  - malfunction of component or operator error
  - should have no safety related consequences to prevent continued reactor operation
- Postulated Accidents
  - probability <10^{-2}/year
  - damage to the plant may occur
  - immediate resumption of operation may not be possible
- Severe Accidents
  - probability <10^{-5}/year
  - severe damage to plant
  - possible radioactive release

Initiating Events requiring calculation of fuel response

Acceptance Criteria

Transient and accident analysis are performed to confirm that the nuclear power plant is capable of coping with the whole set of Anticipated Transients and Postulated Accidents that have been selected as a design basis or as a basis for upgrading without exceeding acceptable limits

Acceptance criteria are mostly aimed to prevent damage to the multiple barriers against uncontrolled release of radioactivity, eg:

- prevention or reduction of clad damage
- limiting number of damaged or failed fuel rods
- maintaining integrity of the primary circuit
- maintaining the integrity of the containment
- direct limitation on the radiological consequence of release

References

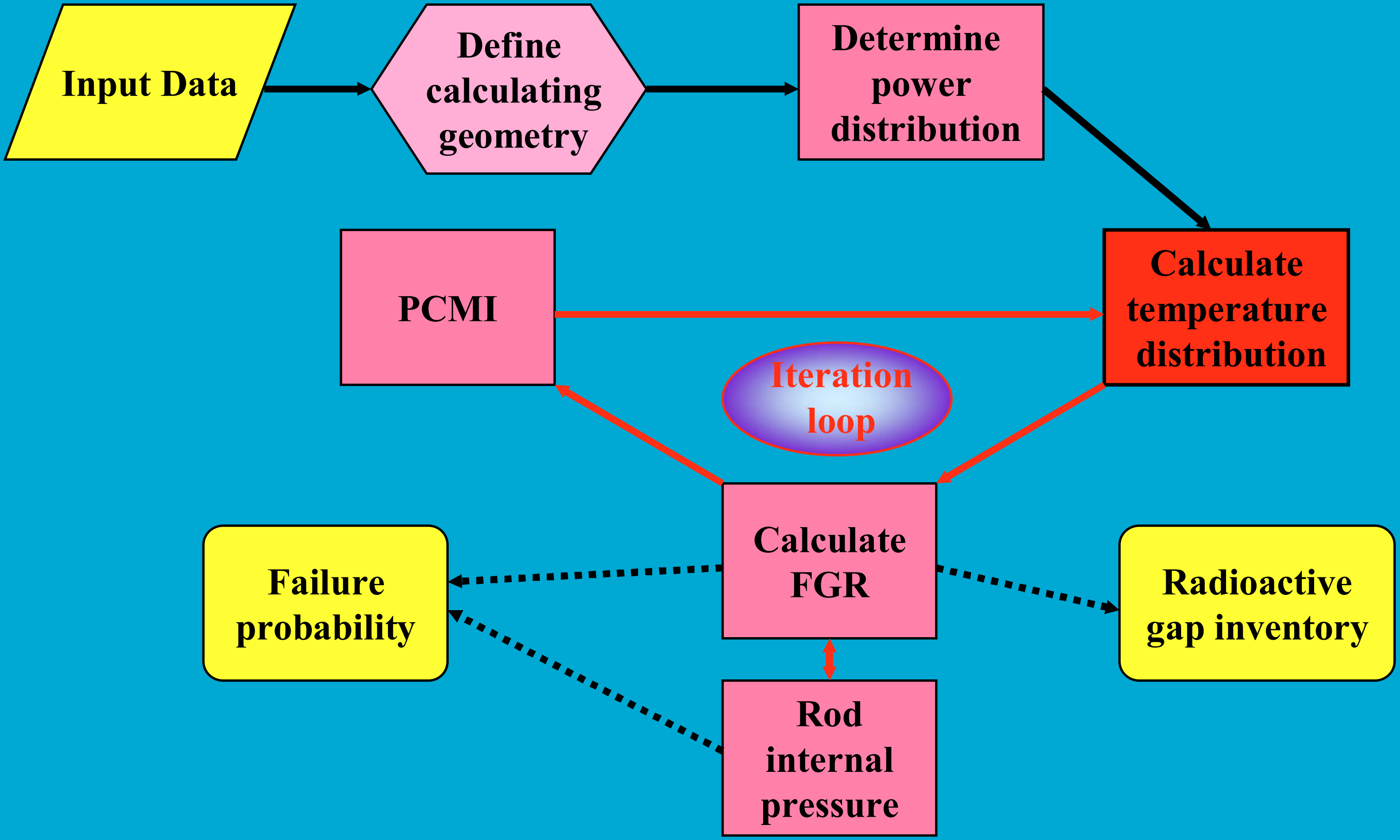
Manual on Quality Assurance for Computer Software Related to the Safety of Nuclear Power Plants
IAEA publication: Technical Report Series No. 282 , Vienna (1988)

Fuel Safety Criteria Technical Review
NEA of the OECD CSNI/R(99)25,OECD, Paris (2001)

Guidelines for Accident Analysis of WWER Nuclear Power Plants
IAEA publication: IAEA-EBP-WWER-01 (December 1995)

Analysis of Differences in Fuel Safety Criteria for WWER and Western PWR Nuclear Power Plants
IAEA publication: IAEA-TECDOC-1381 (November 2003)

Typical code structure


Input Data

Define calculating geometry

Determine power distribution

Calculate temperature distribution

PCMI

Iteration loop

Calculate FGR

Failure probability

Radioactive gap inventory

Rod internal pressure

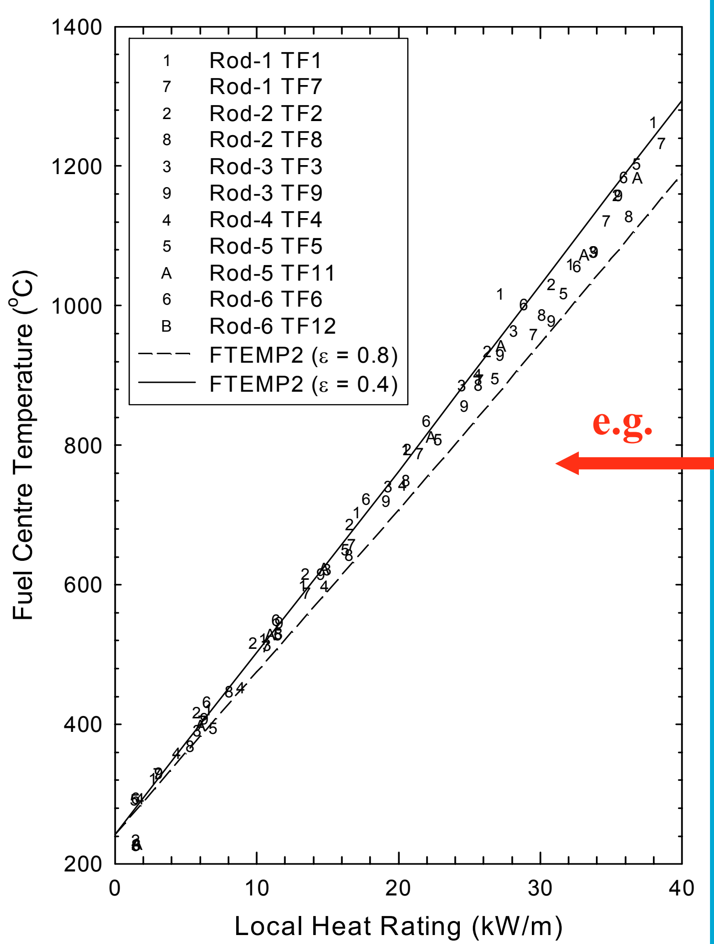
Temperature Calculation

- Coolant-cladding heat transfer
- cladding temperature distribution
- pellet-cladding gap heat transfer

  (conduction through gas, solid-solid contact conduction radiation…………….)
- pellet temperature distribution

  (power distribution, thermal conductivity, fuel porosity, fuel cracking and relocation………….)

Apparent simplicity



e.g.

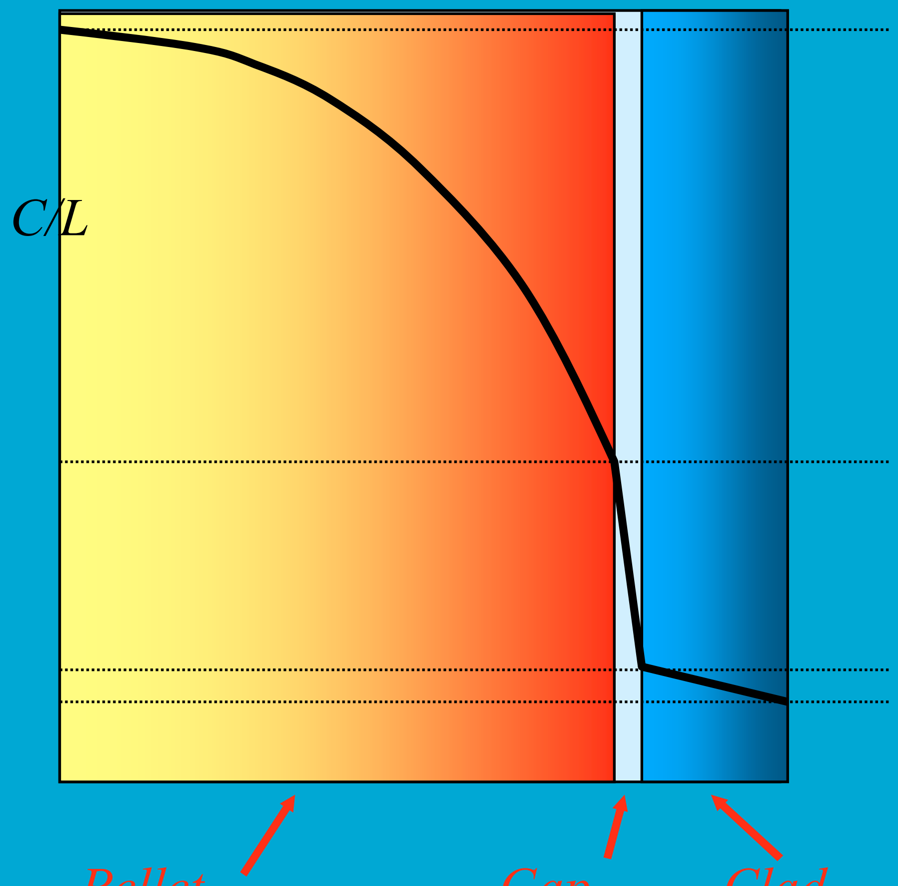
- Cylindrical geometry
- Can measure material properties
  e.g., thermal expansion,
  thermal conductivity etc………
- Have measurements to validate calculations
- Standard solutions to heat flow problems
  good reference is:
  "Conduction of Heat in Solids"
  Carslaw & Jaeger

However, there are a few issues that conspire to make accurate predictions troublesome.

The treatment can be made as complicated or as simple as the modeller wishes.

This presentation will present a pragmatic view serving as an introduction to further reading

Typical temperature distribution @ 20 kW/m



C/L

800 C

430 C

280 C

250 C

Bulk coolant
240 C

Pellet

Gap

Clad

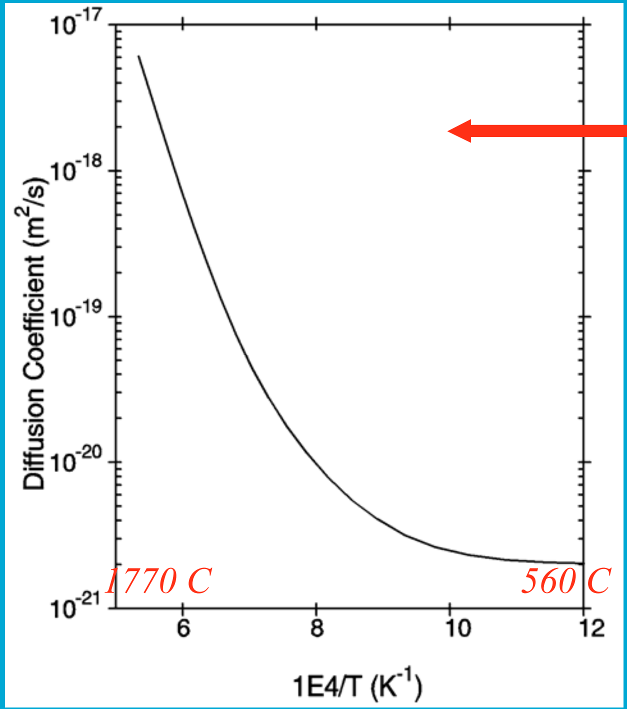
Importance of accurate temperature calculations

- Codes are used for Safety Cases to assess performance of fuel
    - Fuel temperature calculations to show that fuel melting will not occur……….no fuel slumping
    - Calculation of Fission Gas Release (FGR) and rod internal pressure …………no over pressure failures
    - Calculation of Pellet-Clad-Mechanical-Interaction (PCMI) which could lead to mechanical failure of the clad
    - Calculation of radioactive release in the event of clad failure

- UO_2 and MOX have poor thermal conductivities therefore high temperatures even at modest ratings

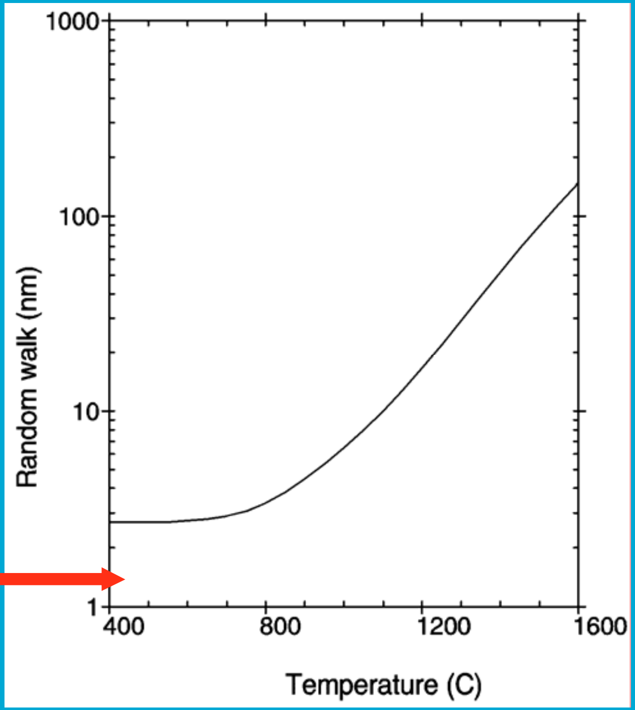
- Many properties are exponentially dependent on temperature therefore accurate temperature estimates are important

Importance of accurate temperature calculations



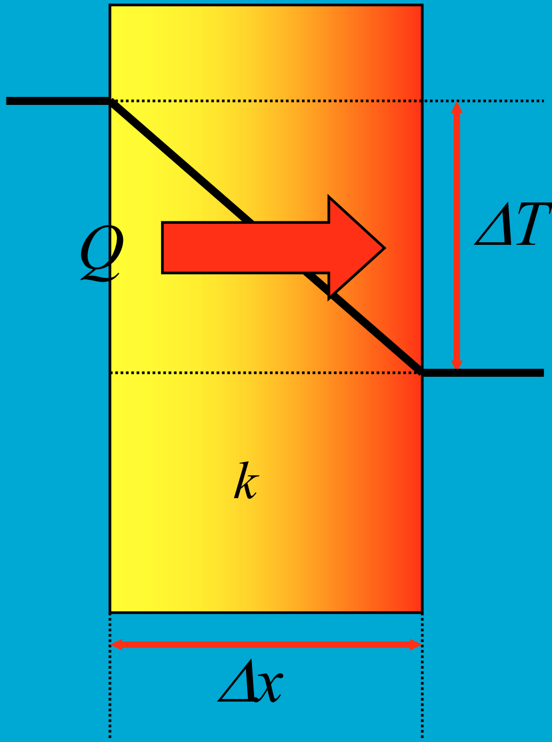
Fission gas atom diffusion coefficient

Atom random walk in one hour



Start at the beginning

……simple heat flow concepts

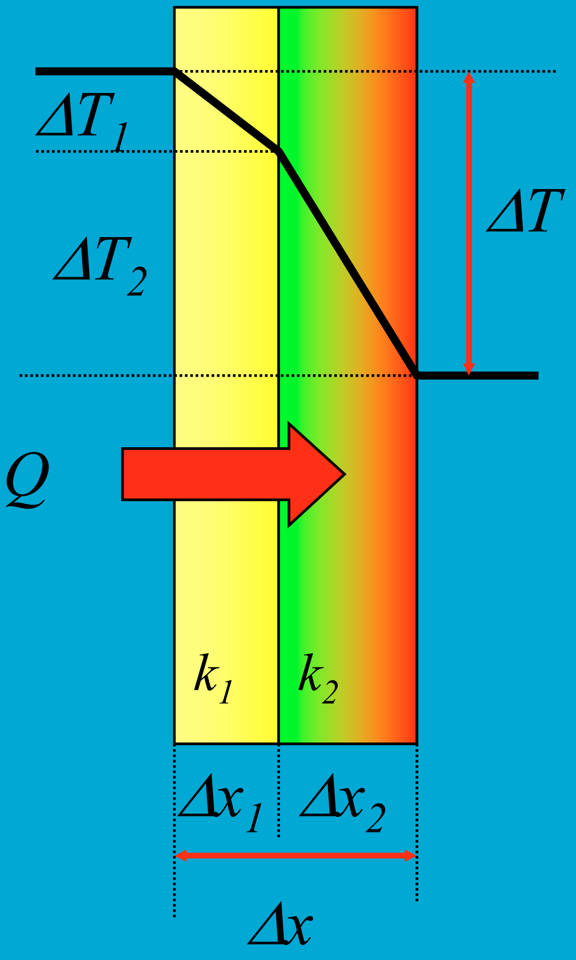


$$Q = k \cdot \frac{\Delta T}{\Delta x}$$

Q	*heat flow per unit area*
$\Delta T/\Delta x$	*temperature gradient*
k	*thermal conductivity,* *typical units W/m/K*
h	*conductance* $= k/\Delta x$
K	*thermal diffusivity* $= k/\rho.SpHt$

Simple heat flow concepts

……..Series conduction



$$\Delta T = \Delta T_1 + \Delta T_2$$

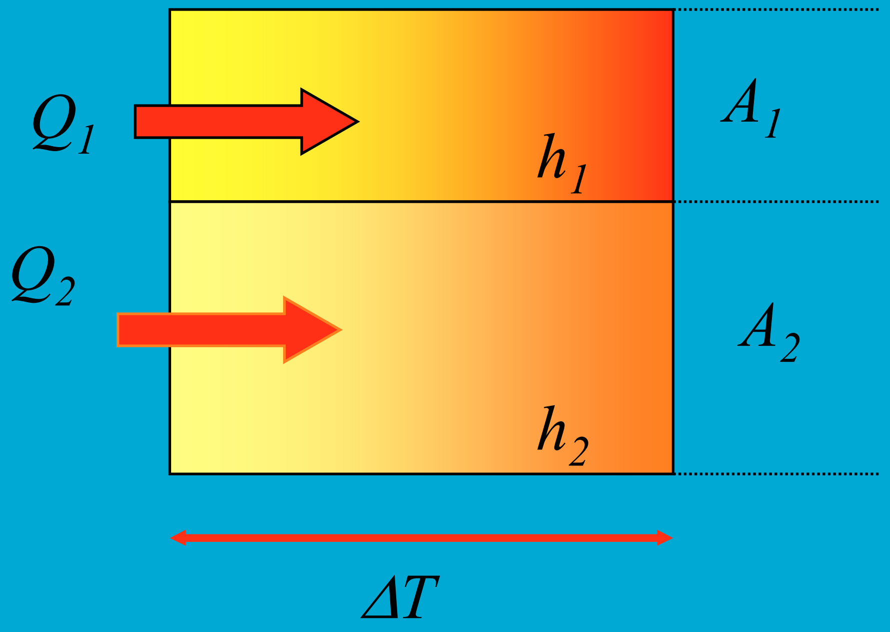
$$\frac{Q}{h} = Q \cdot \left[\frac{1}{h_1} + \frac{1}{h_2}\right]$$

$$\boxed{\frac{1}{h} = \frac{1}{h_1} + \frac{1}{h_2}}$$

$$\boxed{\frac{\Delta x}{k} = \frac{\Delta x_1}{k_1} + \frac{\Delta x_2}{k_2}}$$

Simple heat flow concepts

……..Parallel conduction



$$Q = Q_1 + Q_2$$

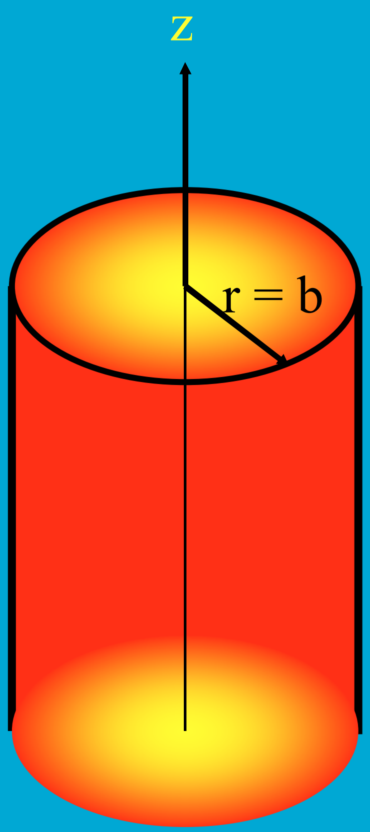
$$\Delta T \cdot h = \Delta T \cdot \left[h_1 + h_2\right]$$

$$\boxed{h = h_1 + h_2}$$

$$\boxed{k = \Delta x \cdot \left[\frac{k_1}{\Delta x_1} + \frac{k_2}{\Delta x_2}\right]}$$

Simple heat flow concepts

…….. Radial heat flow in a cylinder



A_0 = Heat production
per unit vol.

Steady state

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

Hollow cylinder a < r < b

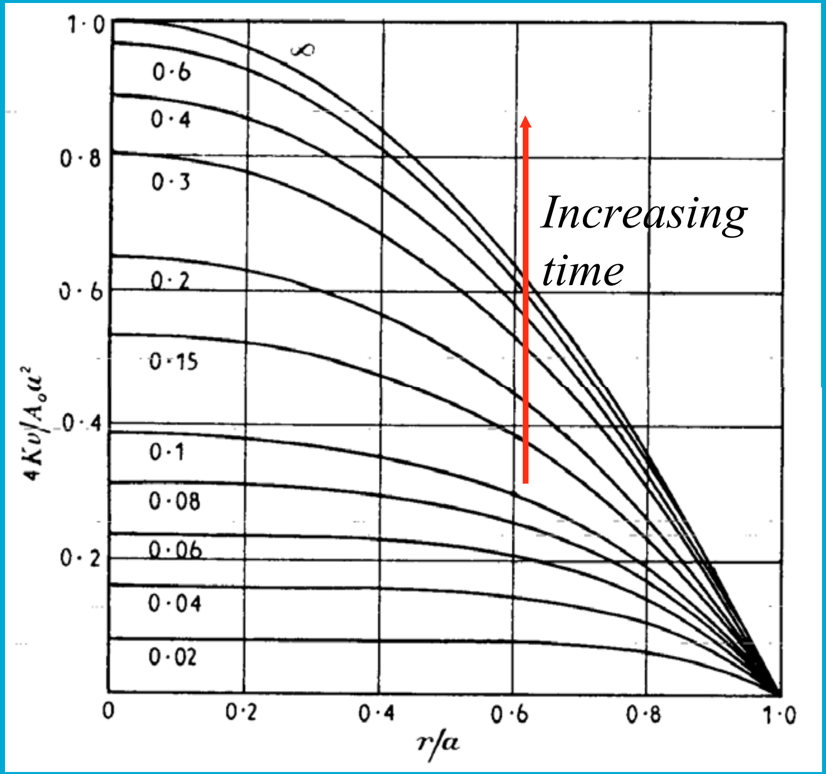
$$T_c = T_s + \frac{A_0}{4k} \cdot \left(b^2 - a^2 \cdot \left(1 - 2\ln\left(b / a\right)\right)\right)$$

Solid cylinder 0 < r < b

$$T_c = T_s + \frac{A_0 \cdot b^2}{4k}$$

Simple heat flow concepts

……..Time dependent sol^{ns}



Equation:

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

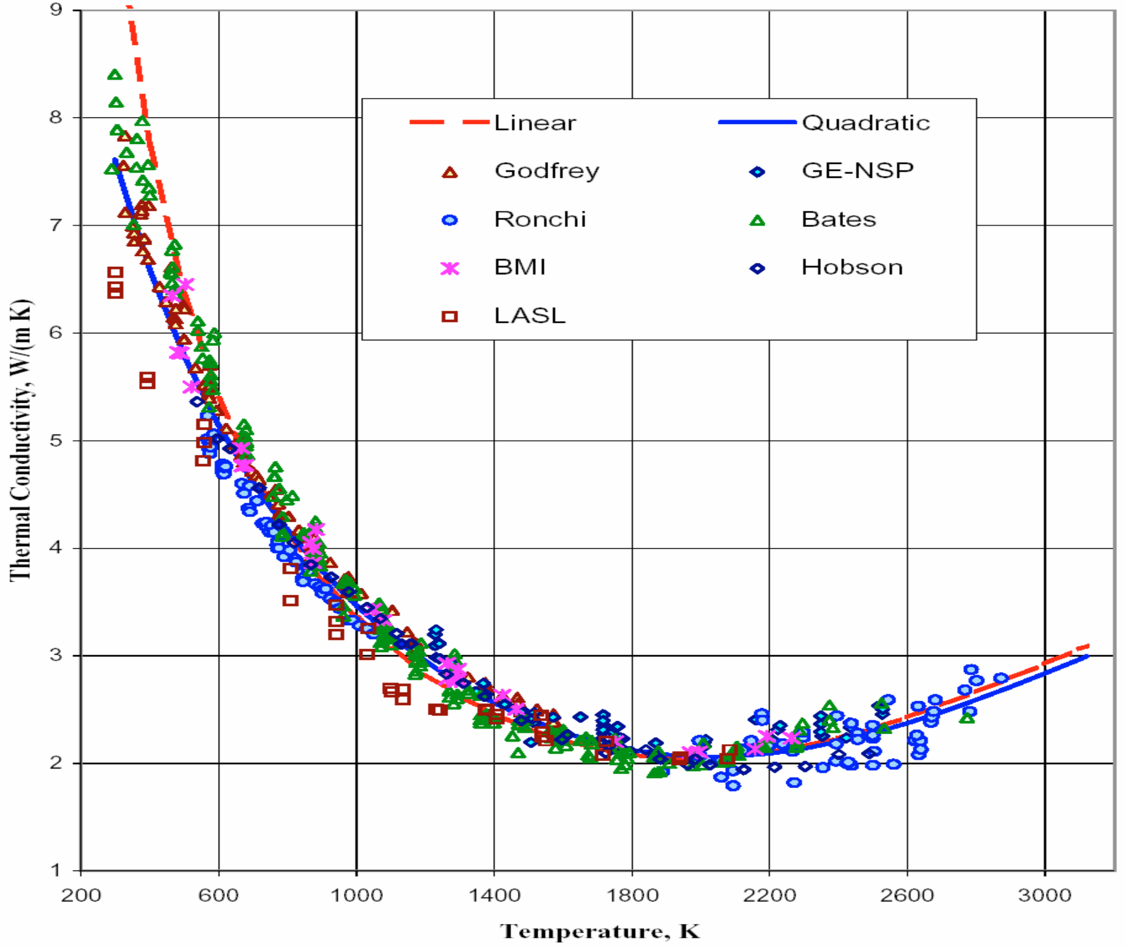
Solution:

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

Bessel functions

Material properties

……..Thermal conductivity

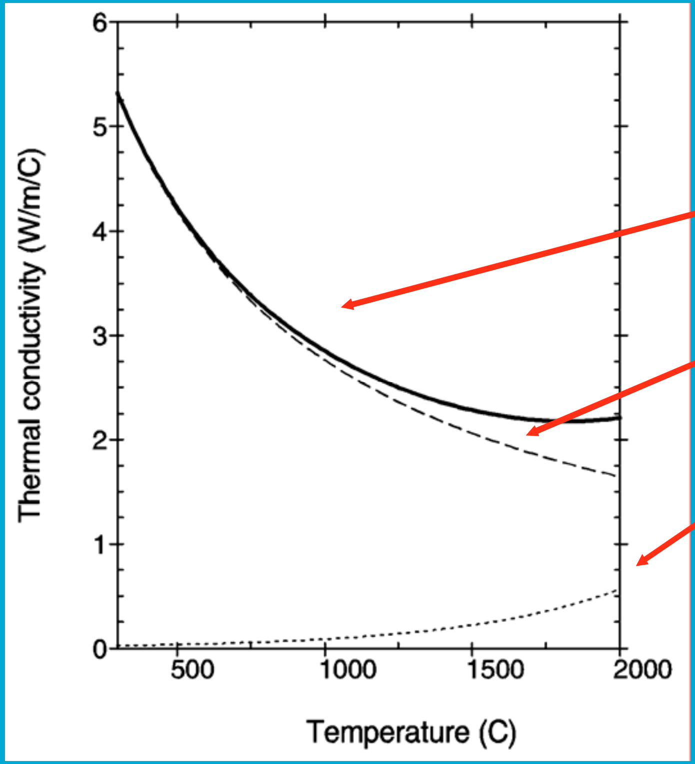


Data for 95% TD UO_2

Material properties

……..Thermal conductivity

95% TD UO_2



$$k = k_{phonon} + k_{electronic}$$

$$k_{phonon} = \frac{1}{A + B * T}$$

$$k_{electronic} = E_1 * \exp(E_2 * T)$$

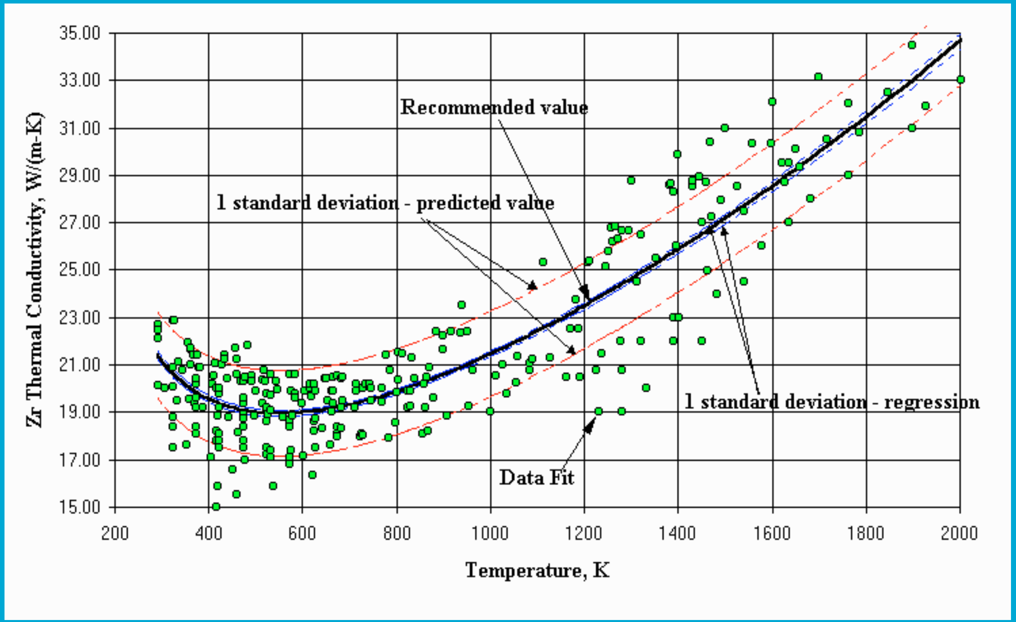
In addition k is dependent on

- porosity
- burn-up
- stoichiometry

Material properties

……..Thermal conductivity

Zircaloy



Over the region of interest

$k = k_{electronic}$

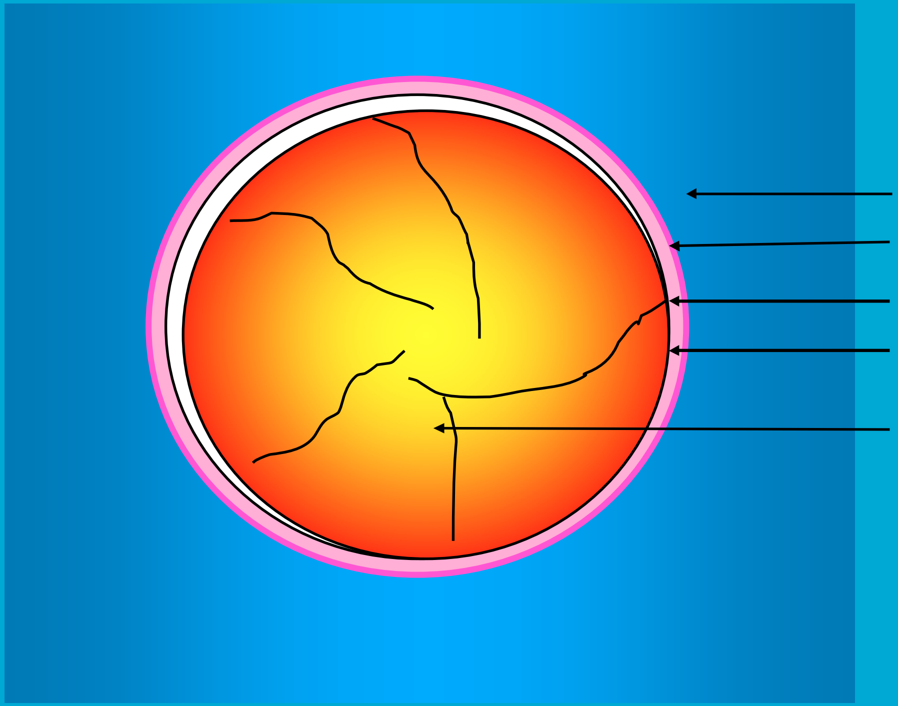
Hence:

$k = E_1 + E_2 * T$

Note: $k_{Zr} >> k_{UO2}$

Modelling fuel temperatures

.........general

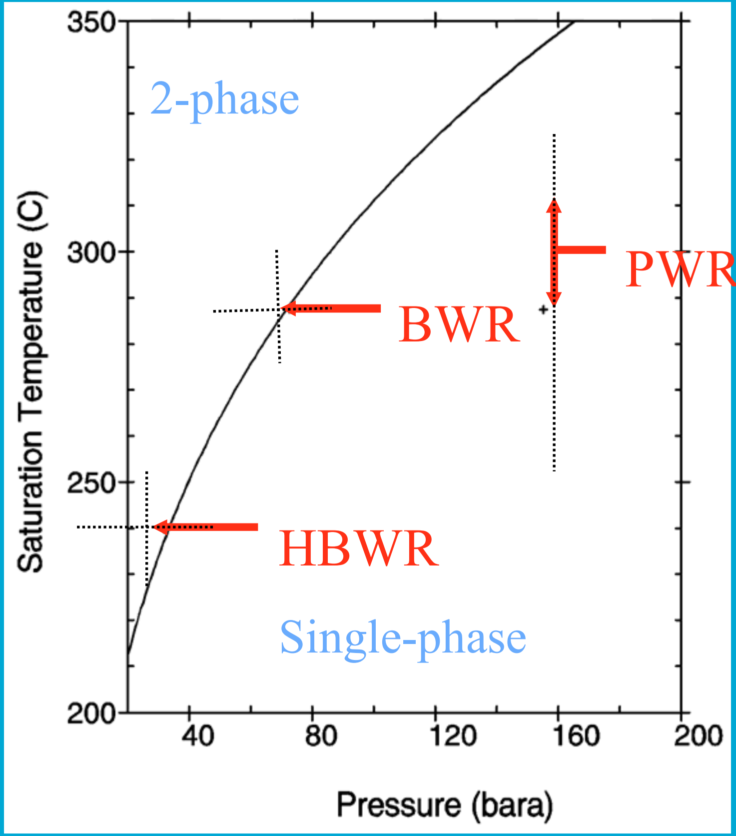


Order of treatment:

1 coolant - oxide heat transfer
2 conduction through oxide
3 conduction through cladding
4 gap conduction
5 conduction through pellet

1 Coolant - oxide heat transfer

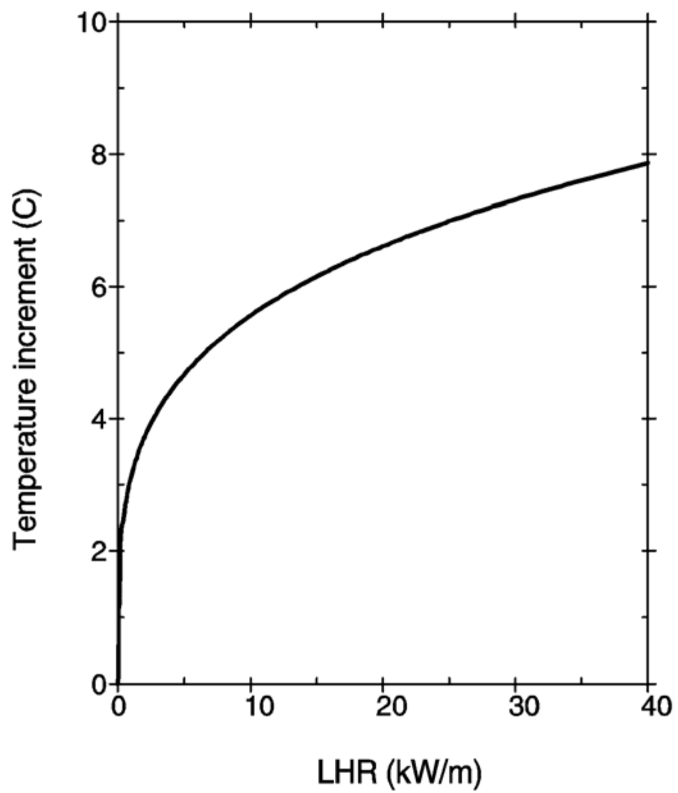
……coolant



Reactor	Pressure	Temperature
HBWR	32 bar	240 C
BWR	72.4 bar	288 C
PWR	155 bar	288 C (inlet)

1 Coolant - oxide heat transfer

……BWR



Jens-Lottes Correlation

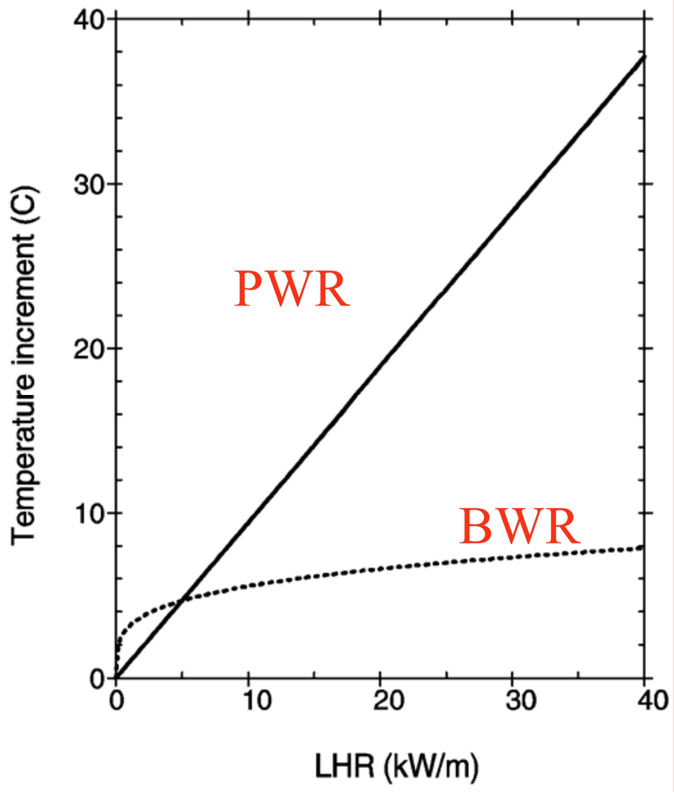
- Unique relation between ΔT, and heat flux at a given system pressure
- For a commercial BWR:

$$\Delta T = 1.040 * \left(\frac{LHR\,(kW\ /\ m)}{DCO\,(m)} \right)^{0.25}$$

Clad O/D

1 Coolant - oxide heat transfer

……PWR

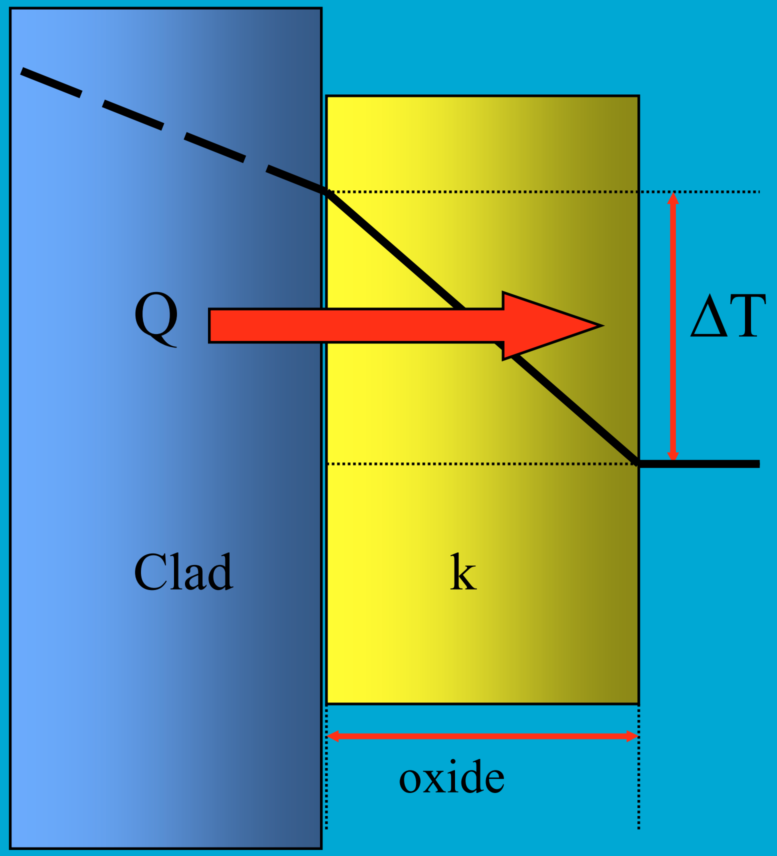


Dittus-Boelter Correlation

- more complicated than BWRs
- bulk coolant temperature increases up channel
- outlet temperature in commercial PWR ~30 C higher than inlet temperature

2 Conduction through oxide layer

……



- Layer thickness < 100 microns
- can be treated in 1 dimension
- k ~ 2 W/m/K

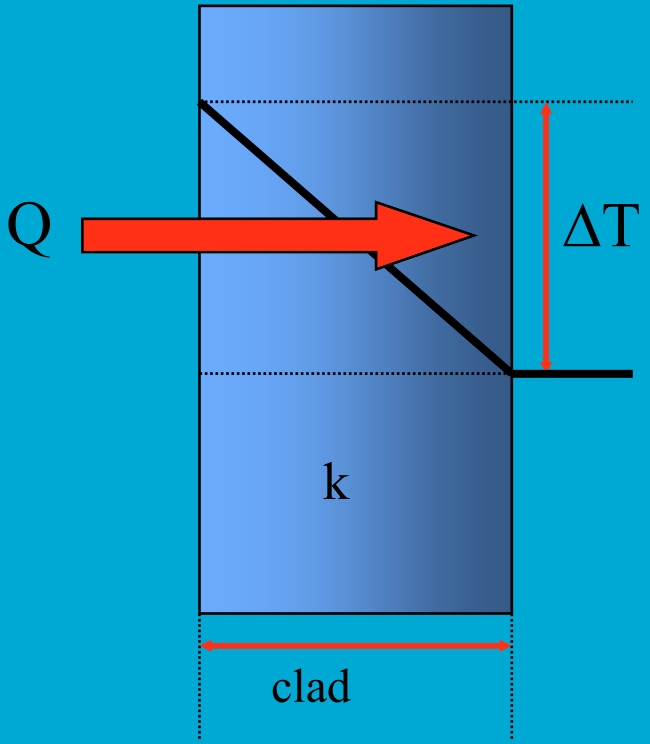
Example: ΔT for 10 microns of
oxide at 40 kW/m?

ΔT ~ 5.9 C

Rule of thumb:
At 20 kW/m, ΔT ~ 0.3 C/micron

3 Conduction through clad

……



- wall thickness ~0.6 - 0.9 mm can be treated in 1 dimension
- k ~ 20 W/m/K

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

ΔT ~ 19 C

4 Gap Conduction

……

3 parallel conduction routes:

- by radiation
- through areas of contact
- through the gas gap

$$h_{total} = h_{radiation} + h_{contact} + h_{gas}$$

4 Gap Conduction

……….. radiation

Stefan’s constant

Mid gap temperature (K)

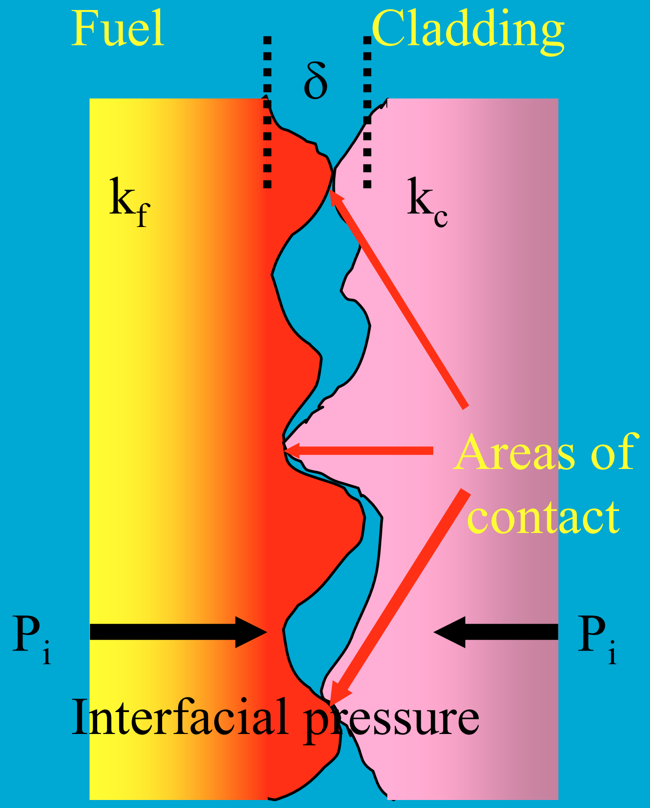
$$h_{radiation} = \frac{4 \cdot \sigma \cdot T^3}{(1/\varepsilon_f) + (1/\varepsilon_c) - 1}$$

Fuel & clad emissivities

- Small contribution under normal operations
- no dependence on gap size

4 Gap Conduction

……….through areas of contact



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

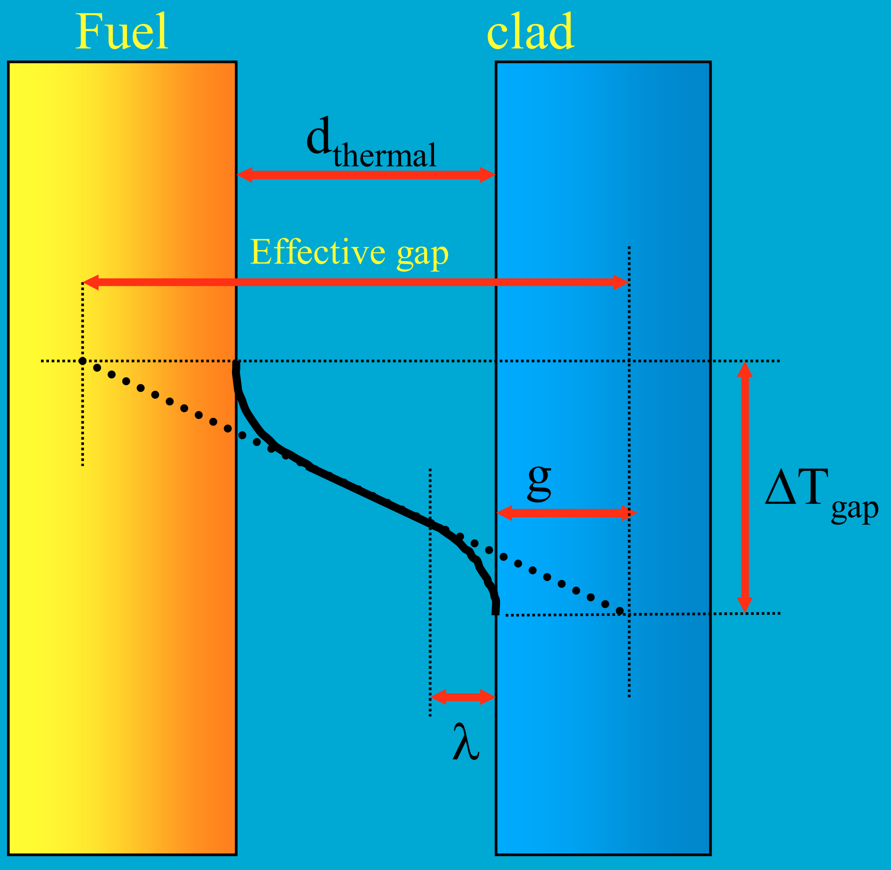
$$h_{contact} = Const \cdot \left(\frac{2k_f k_c}{k_f + k_c} \right)^{\beta} \cdot \frac{P_i}{\delta^{1/2} \cdot H}$$

Fitted to data

Meyer hardness

4 Gap Conduction

……….through gas gap



Imperfect heat transport across solid-gas interface leads to the concept of a:

“Temperature Jump Distance” (g)

which effectively increases the gap size:

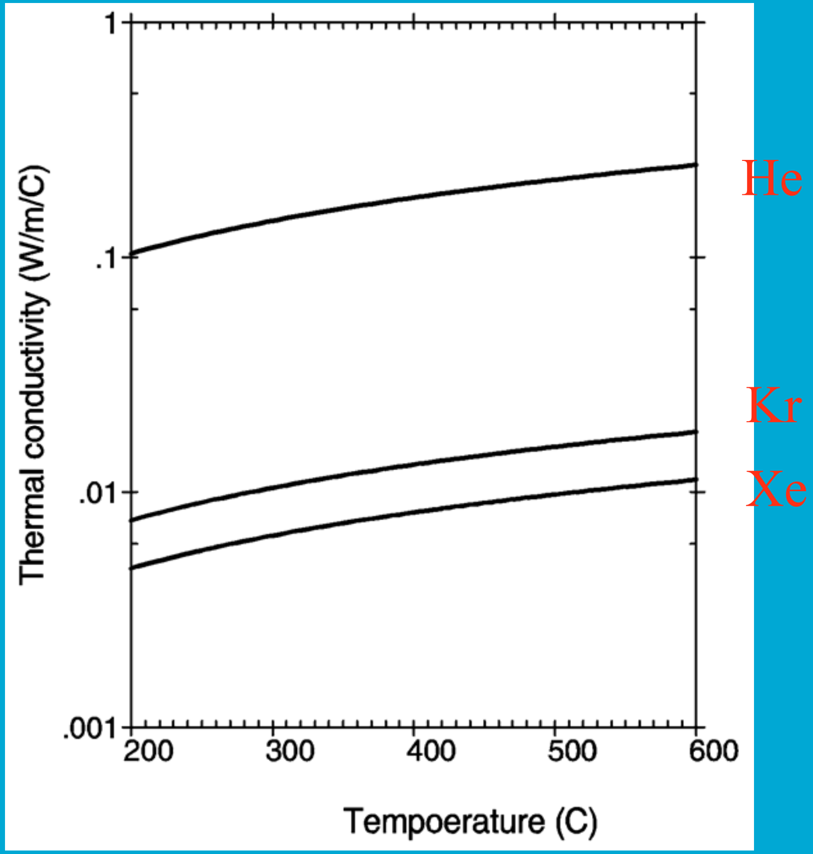
$$h_{gas} = \frac{k_{gas}}{\delta + d_{thermal} + 2g}$$

Surface roughness

Temperature jump distance

4 Gap Conduction

…….Gas conductivity



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

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

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

4 Gap Conduction

…….temperature jump distance

Imperfect heat transport across solid-gas interface, Kennard from kinetic theory of gases gives:

$$g = \left(\frac{2-a}{a}\right) \cdot \frac{4 \cdot Const}{(\gamma + 1)} \cdot \frac{k_{gas}}{\eta C_v} \cdot l$$

a	accommodation coefficient
Const	~ 2
γ	C_p/C_v
η	viscosity
l	mean free path

4 Gap Conduction

……. Accommodation coefficient

For collision between molecules, Kinetic Theory of gases gives:

$$a = \frac{2mM}{(m + M)^2}$$

For collision between gas (M) and solid molecule $a_x b_y$:

$$a_M = \frac{4M}{x m_a^{2/3} + y m_b^{2/3}} \left[\frac{x m_a^{5/3}}{(M + m_a)^2} + \frac{y m_b^{5/3}}{(M + m_b)^2} \right]$$

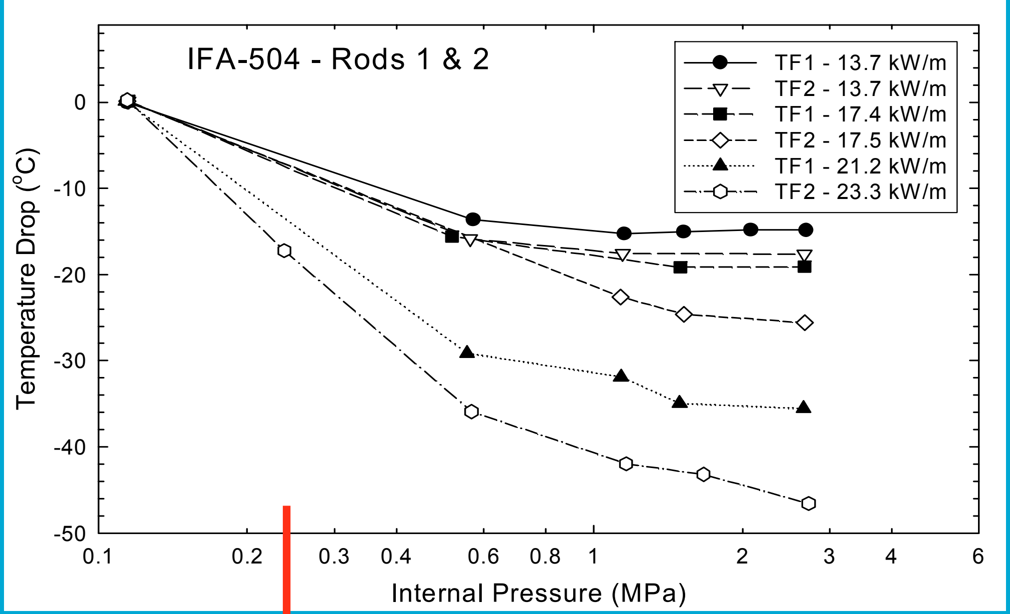
Pragmatically, Lanning & Hann give for the rare gases:

$$a_M = (a_{Xe} - a_{He}) \frac{M - 4}{128} + a_{He}$$

a_{He} ~0.35, a_{Xe}~1 for UO_2/Zr (Giulaini & Mustacchi data)

4 Gap Conduction

…….temperature jump distance



In terms of measurable quantities,

Lanning & Hann give:

$$2g = \frac{2 \cdot Const \cdot k_{gas}\sqrt{T} \cdot fu(gas)}{P_{gas}}$$

Assuming $k_{gas}=AT^s$

$$2g = \frac{2g_0(T/273)^{s+0.5}}{P_{gas}}$$

$\boxed{2g_0 \sim 4.5 \pm 0.5\ \mu m}$

STP value

4 Gap Conduction

…….temperature jump distance

The Halden FTEMP code uses the following empirical expression :

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

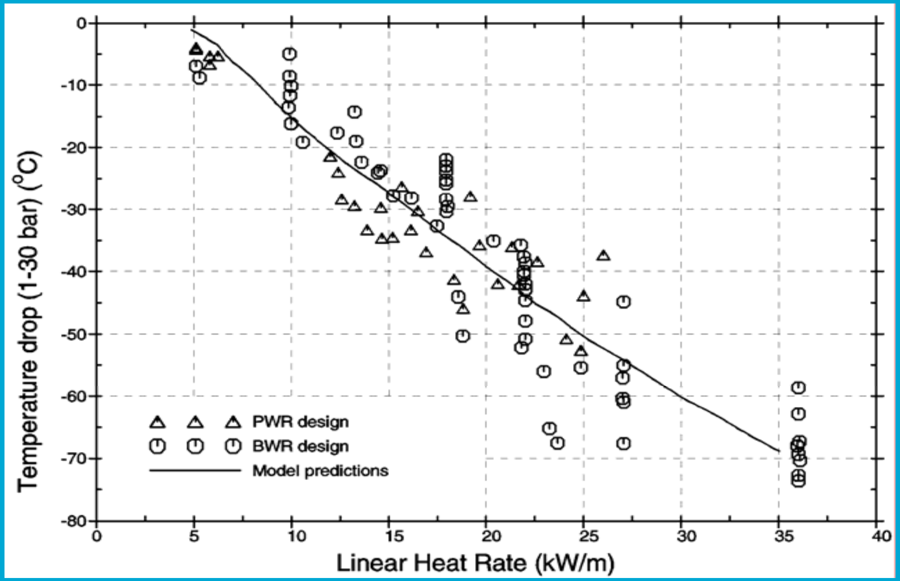
x_{Xe}	fraction of Xe in He
P	gas pressure (ata)

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

~6 .6 µm	He
~0.66 µm	Xe

4 Gap Conduction

…….temperature jump distance



A Dilemma!

Gates & White found different values of g_0 when applying the same methodology to rods of different diameter - BWR & PWR.

Rationalized results with expression:

$$2g_0 = \frac{r_{out}}{Q}\cdot(f \cdot T - e)$$

Where constants
f = 2.5.10^{-2}
e = 13.44

Pragmatic but something is wrong with theory!

4 Gap Conduction

…….thermal gap - $d_{thermal}$

At beginning-of-life the value of the fuel -to-clad gap is estimated from:

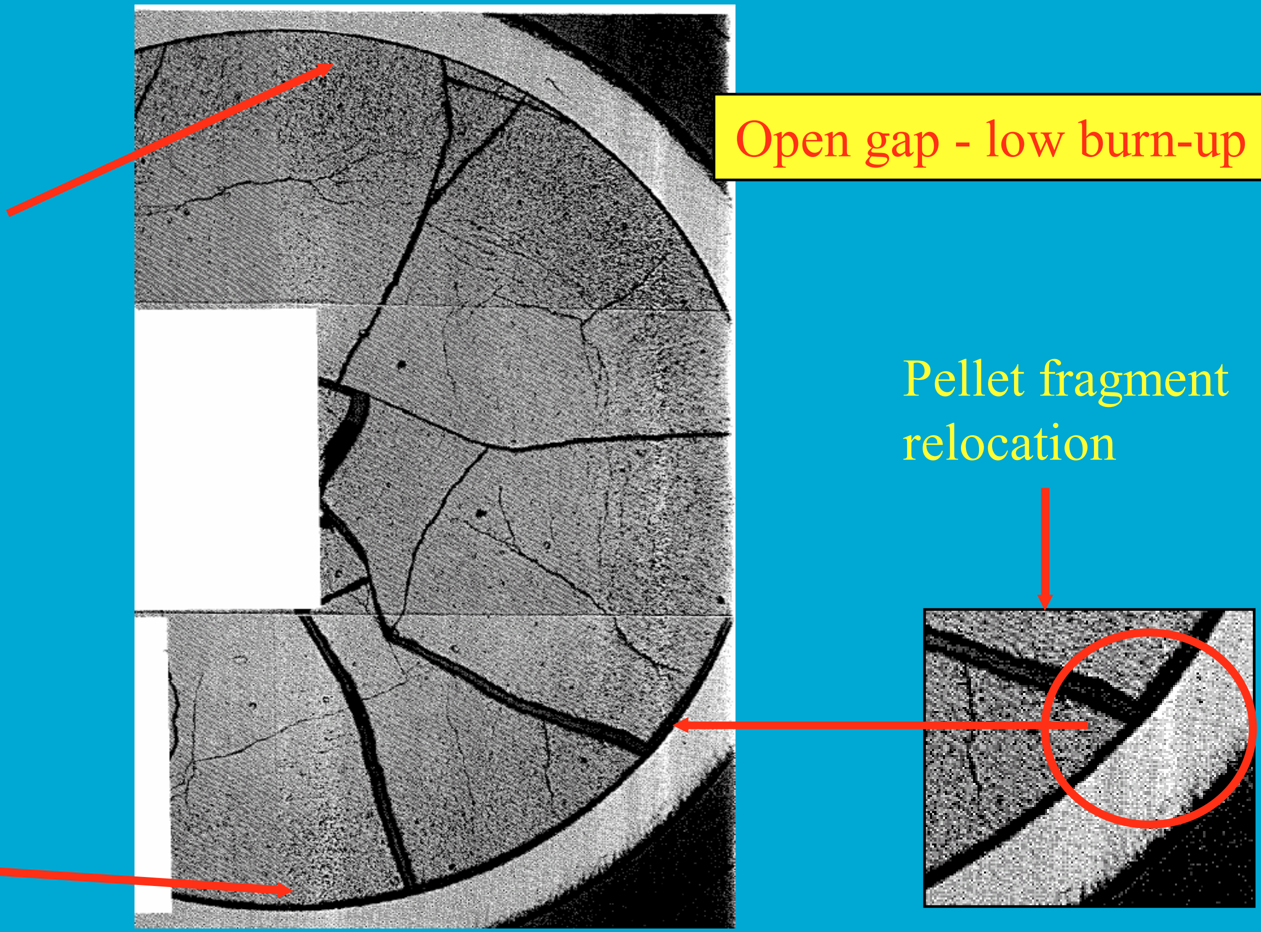
- manufactured dimensions
- thermal expansion

Also, account must be taken of:

- pellet cracking and fragment relocation
- densification
- swelling

4 Gap Conduction

……pellet cracking and fragment relocation



Area of contact

Eccentric pellet

Open gap

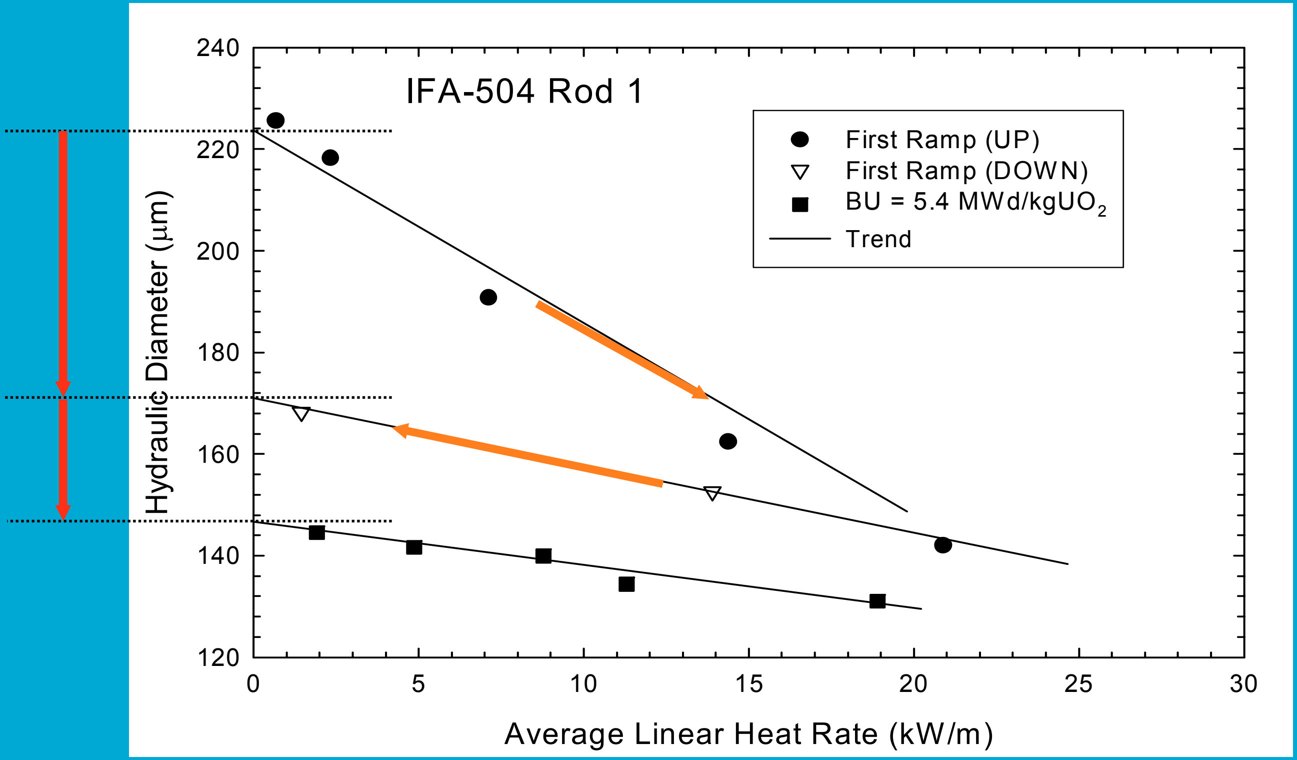
Open gap - low burn-up

Pellet fragment relocation

4 Gap Conduction

……pellet cracking and fragment relocation

Gap closure by:

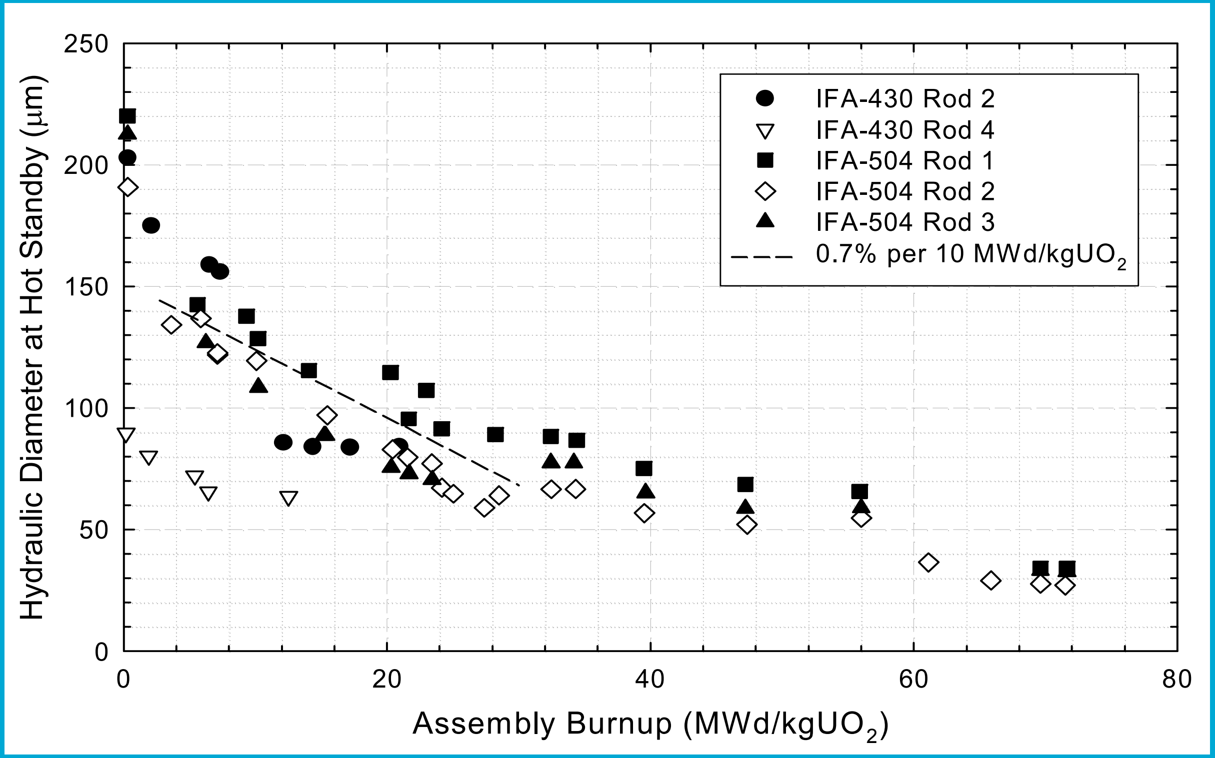


Pellet fragment relocation

Fuel swelling

4 Gap Conduction

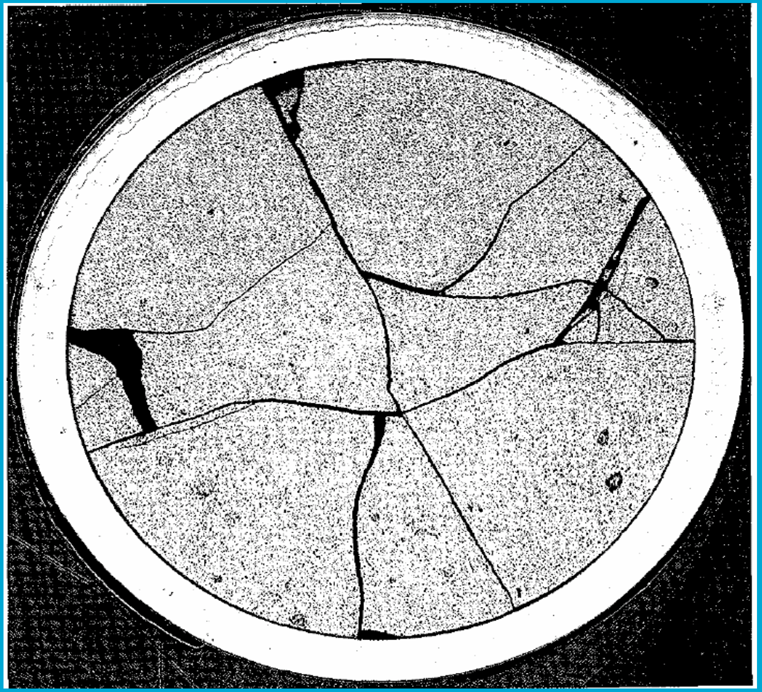
……fuel swelling



$\Delta V/V = 0.5 - 1\%$ *per* 10 *MWd/kgUO*$_2$

4 Gap Conduction

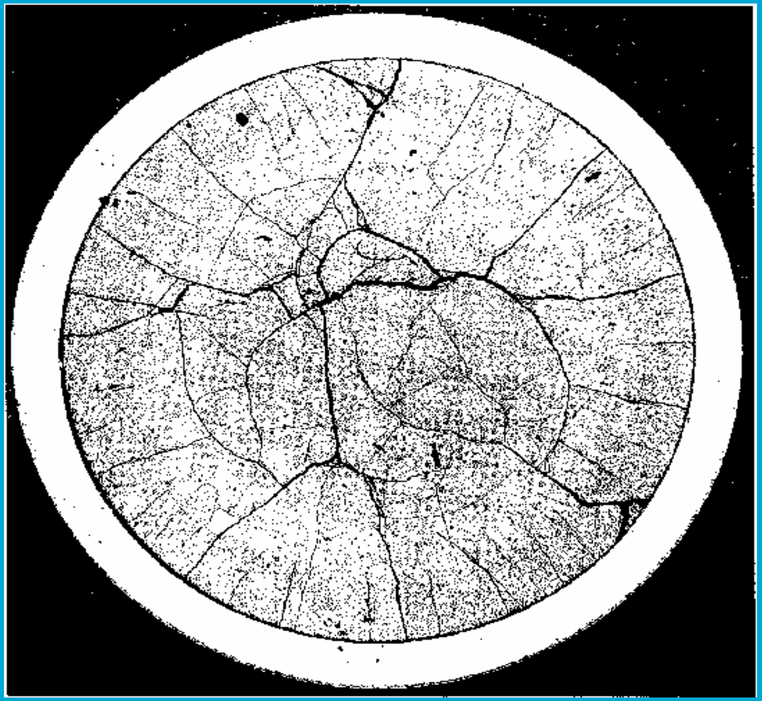
…….pellet cracking



Low power
few cracks

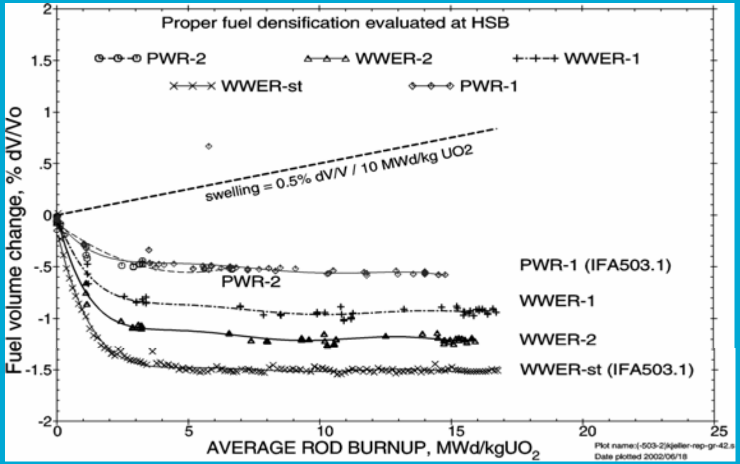
Ramped to high power
many cracks

High burn-up - closed gap



4 Gap Conduction

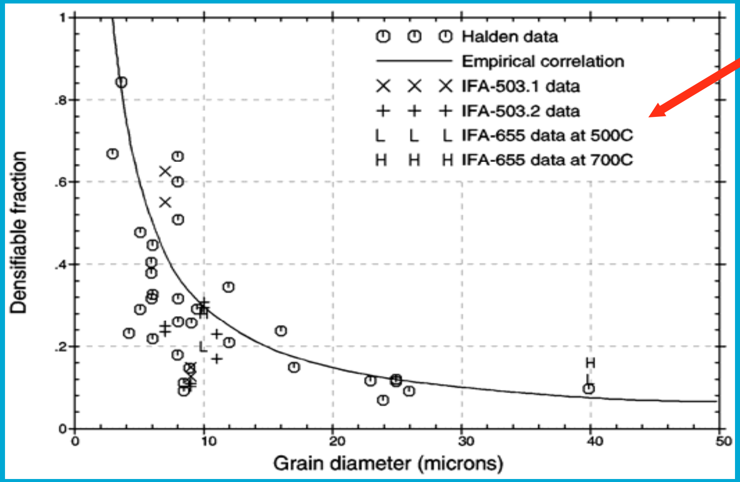
…….densification

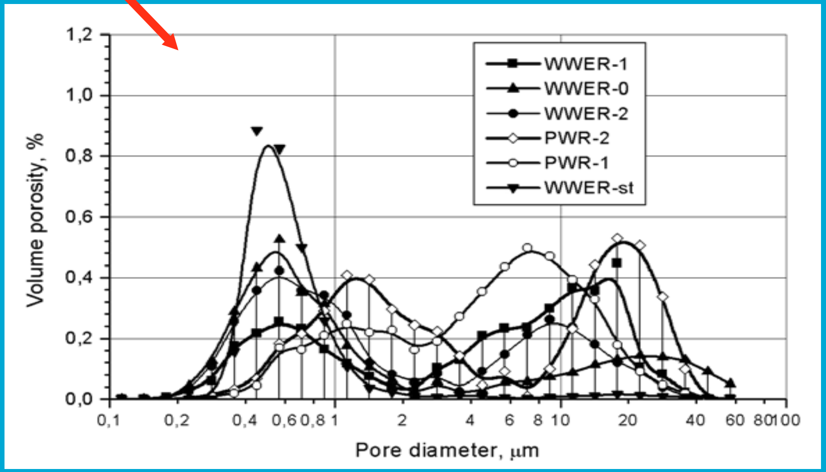


Empirical correlation with grain size, (White)

But

densification depends on pore size distribution particularly <1 μm

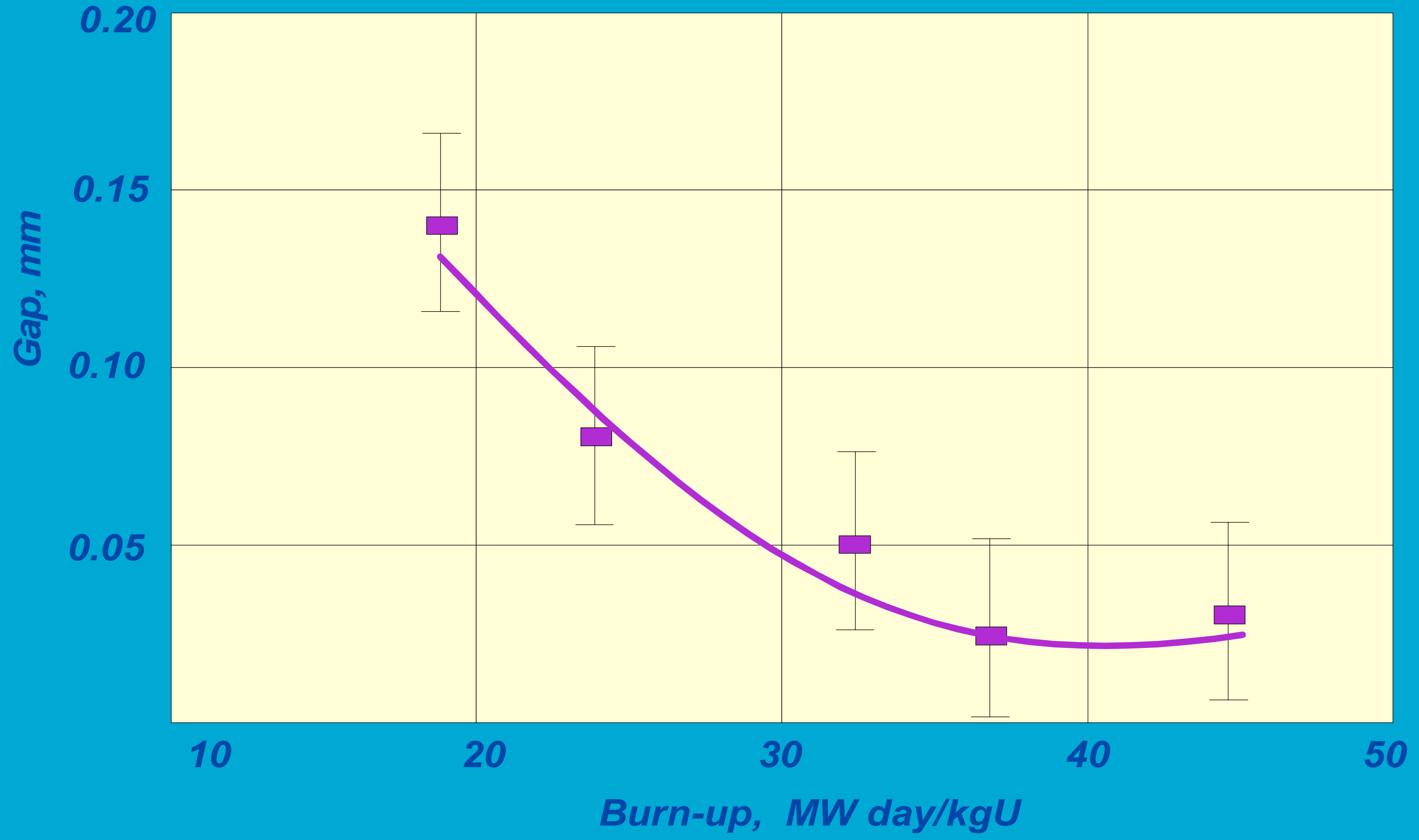




4 Gap Conduction

…….gap closure

Gap between "fuel pellet - cladding"



4 Gap conduction

…….model formulation

Different approaches, e.g:

$$h = h_{rad} + h_{cont}(P) + \frac{k_g}{\delta + 2g + d \cdot \theta_{reloc}}$$

or

$$h = h_{rad} + h_{cont}(P) + \frac{k_g}{\delta + 2g + (d - d_{reloc})}$$

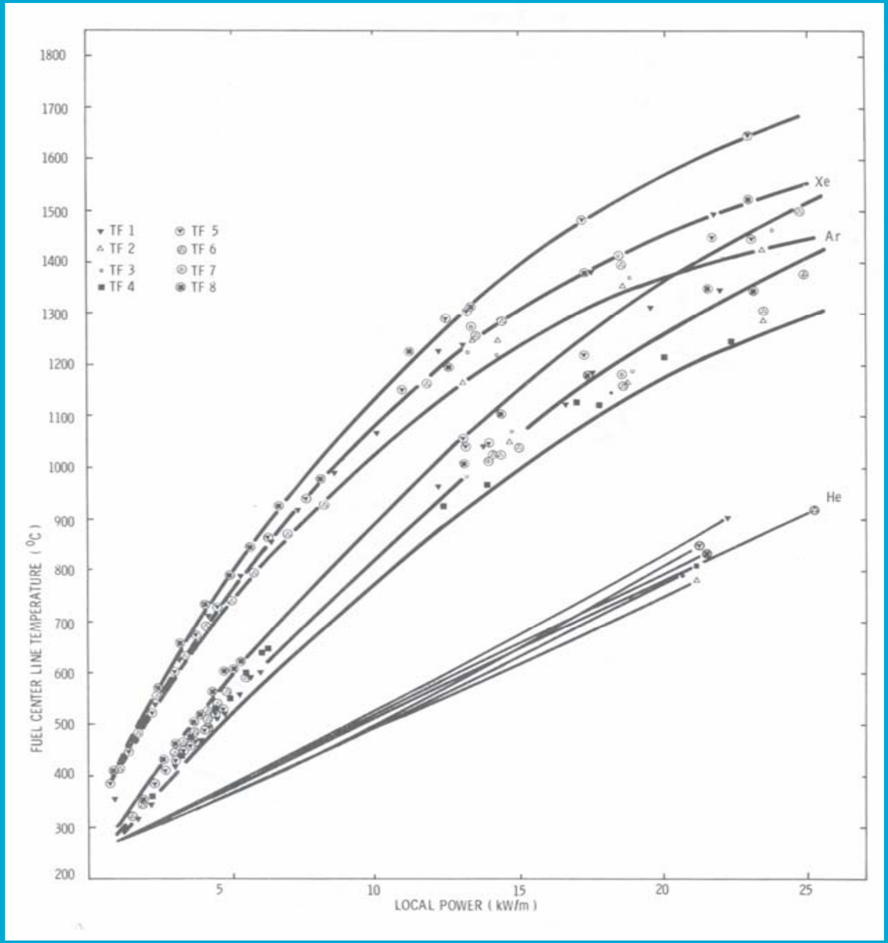
or

$$h = h_{rad} + x \cdot f(h_{gas}) + (1 - x) \cdot f(h_{cont})$$

No model has been shown to outperform all others

4 Gap conduction

…….model formulation



Xe
A

He

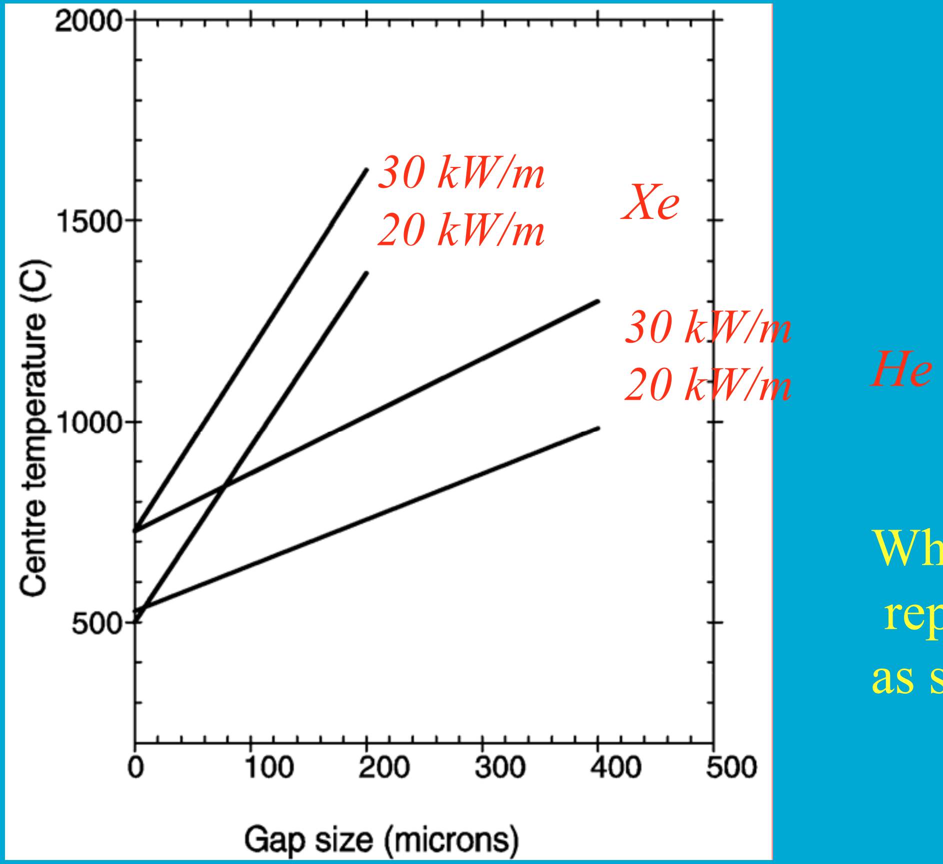
What ever the model, it should reproduce this kind of behaviour as measured in a Halden tests

Note the spread in measurements due to the stochastic nature of pellet fragmentation and relocation

This places a fundamental limit on the expected accuracy of predictions

4 Gap conduction

…….model formulation



What ever the model, it should
reproduce this kind of behaviour
as synthesized from Halden tests

5 Conduction through pellet

…….thermal conductivity

The two common formulations of the phonon term are:

$$k_1 = \frac{1}{A + B \cdot T}$$

Which can be extended to include point defect scattering

$$k = \frac{1}{A_0 + \sum A_i \cdot C_i + B \cdot T}$$

e.g. burn-up Bu:

$$k = \frac{1}{A_0 + A_1 \cdot Bu + B \cdot T}$$

5 Conduction through pellet

…….thermal conductivity

and $$k = \frac{k_1}{x} \cdot \arctan(x)$$

$$where$$

$$x = D \cdot \sqrt{\Gamma} \cdot \sqrt{k_1}$$

$$and$$

$$x = \sqrt{\sum x_i^{\,2}}$$ For multiple scattering types

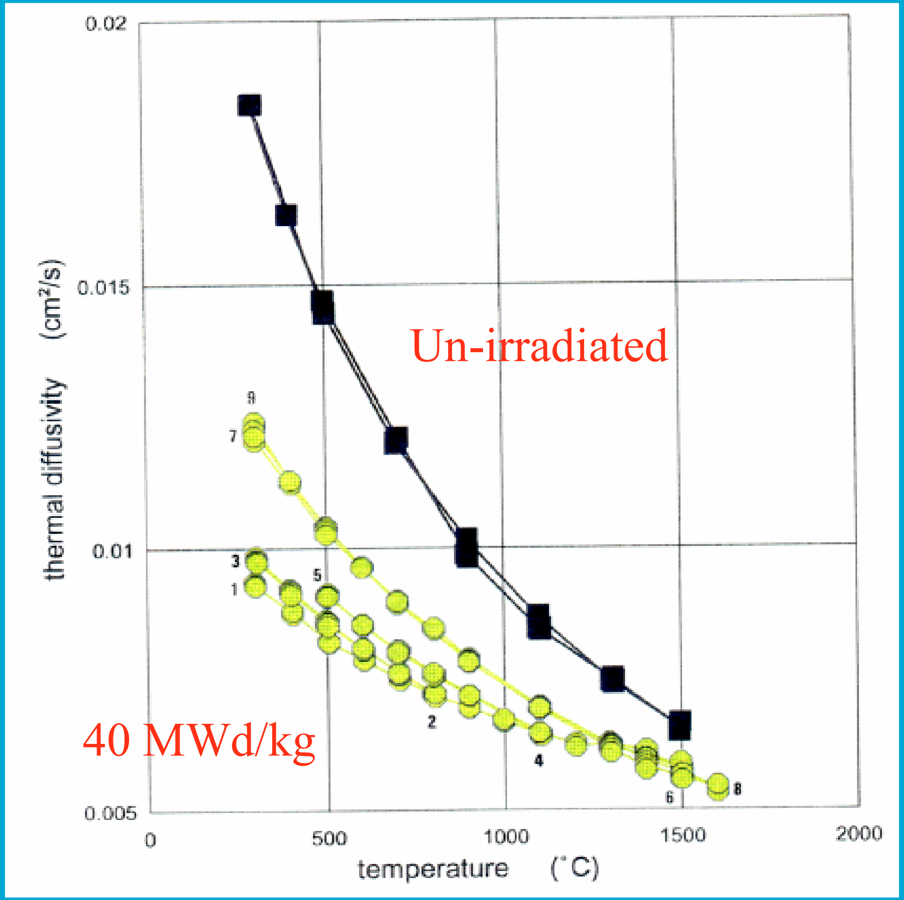
e.g. for burn-up, Γ = Bu

$$k = \frac{\sqrt{k_1}}{D\sqrt{Bu}} \cdot \arctan(D \cdot \sqrt{Bu}\sqrt{k_1})$$

Formulations agree for zero and low burn-up, but diverge at high burn-up

5 Conduction through pellet

…….thermal conductivity

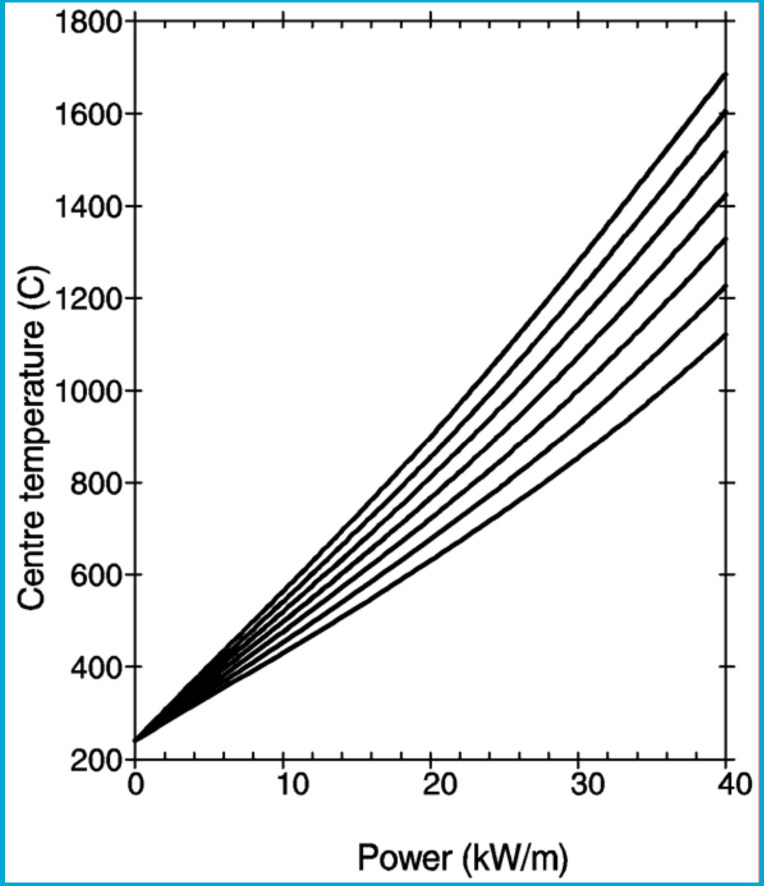


The effect of burnup as measured using laser flash

thermal diffusivity = k/ρ.SpHt

5 Conduction through pellet

…….thermal conductivity

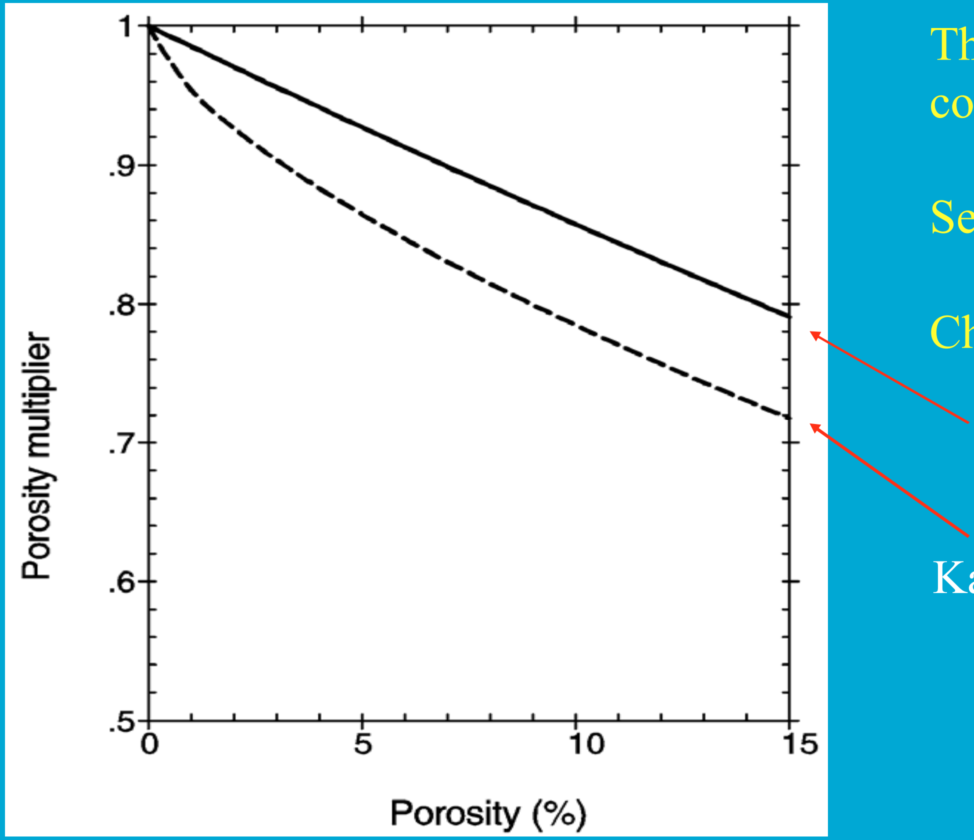


60 MWd/kgUO_2
50
40
30
20
10
0

Effect of burn-up on the centre temperature of a BWR design rod in HBWR

5 Conduction through pellet

…….thermal conductivity



The effect porosity P is to reduce the conductivity.

Several different formulations exist, e.g.:

Christensen

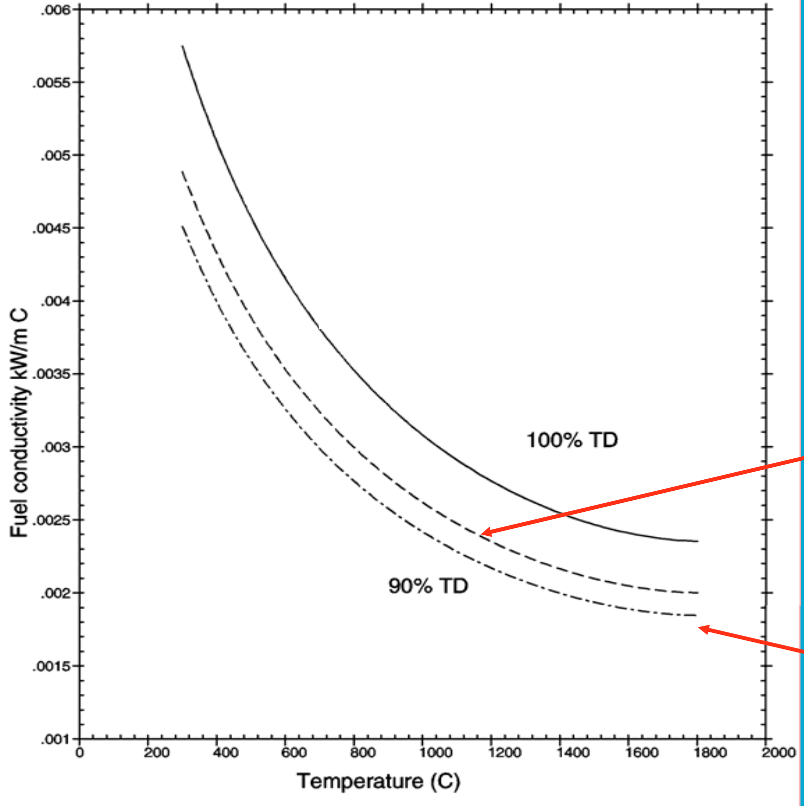
$$k(P) = \frac{k(100\%) \cdot (1 - P)}{(1 + P / 2)}$$

Kampf & Karsten

$$k(P) = k(100\%) \cdot (1 - P^{2/3})$$

5 Conduction through pellet

…….thermal conductivity



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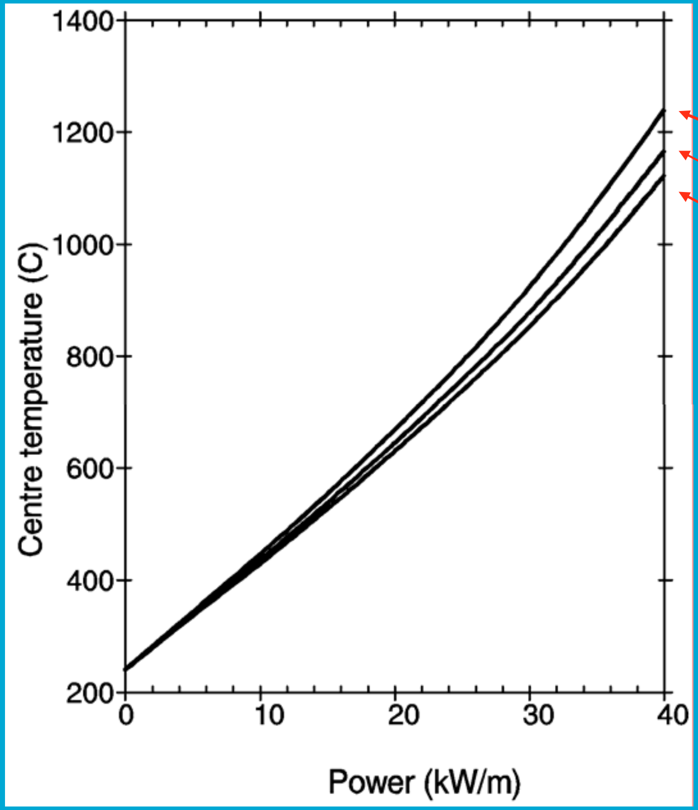
5 Conduction through pellet

…….thermal conductivity

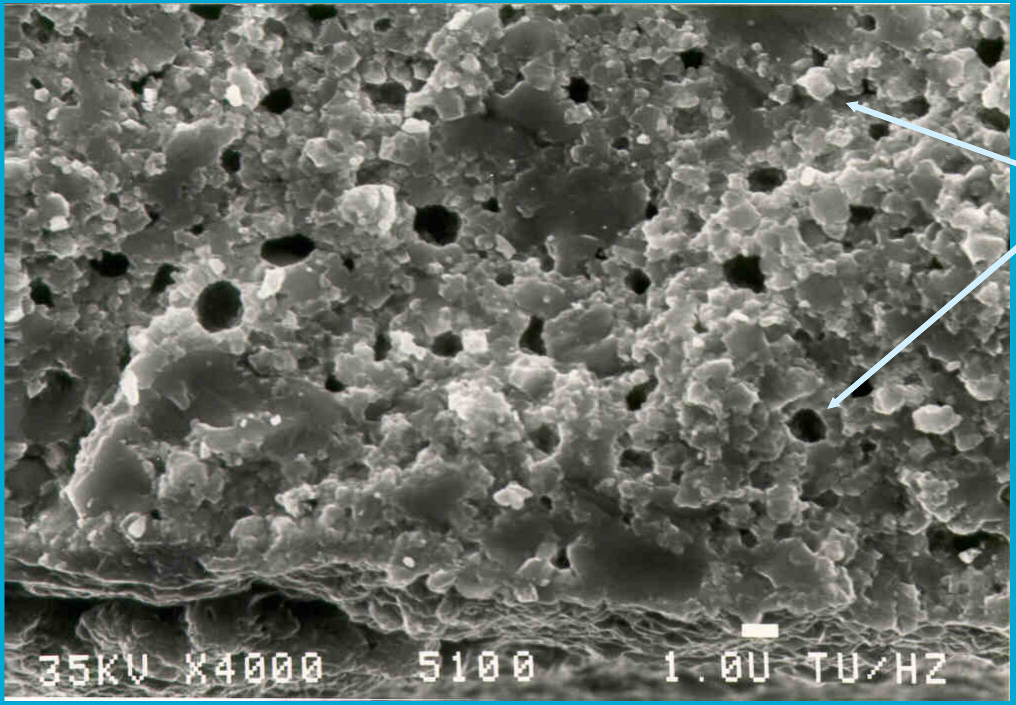


The effect porosity P is to reduce the conductivity.

90% TD
93% using the Christensen correlation
95%

5 Conduction through pellet

…….thermal conductivity



At very high burn-up >60 MWd/kg fuel restructures to form

- very small grains (0.1 - 0.2 µm)
- 1 µm diameter pores
- reduced matrix Xe

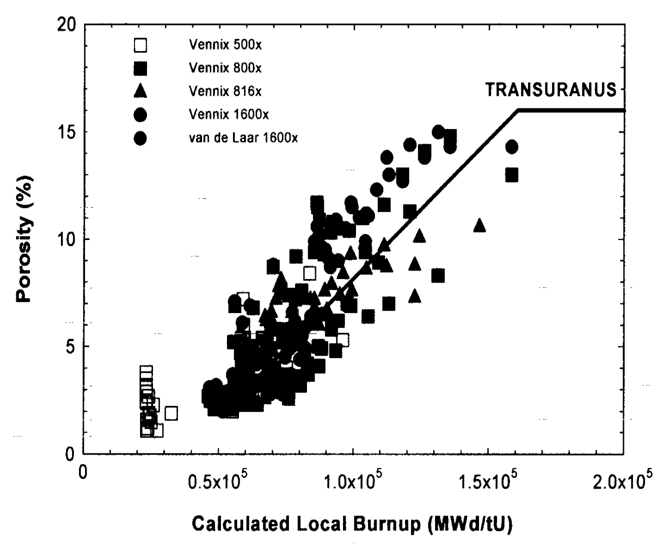
This occurs first at the pellet rim and affects pellet conductivity

Need a model for

- rim thickness
- porosity
- conductivity

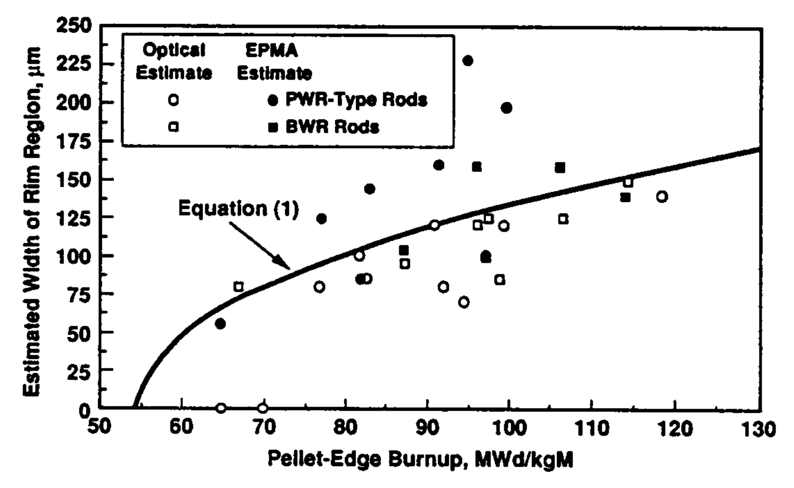
5 Conduction through pellet

…….effect of rim



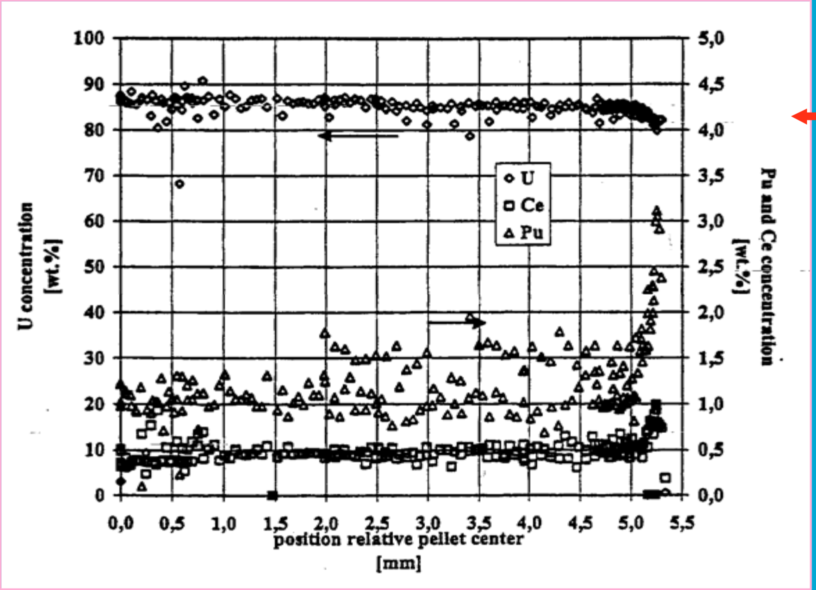
measured porosity

Measured rim thickness



5 Conduction through pellet

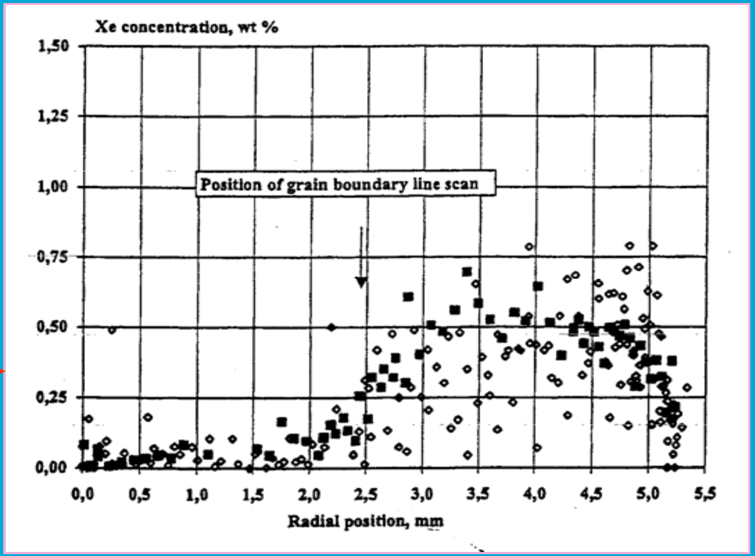
…….effect of rim



measured concentrations, U, Cs & Pu

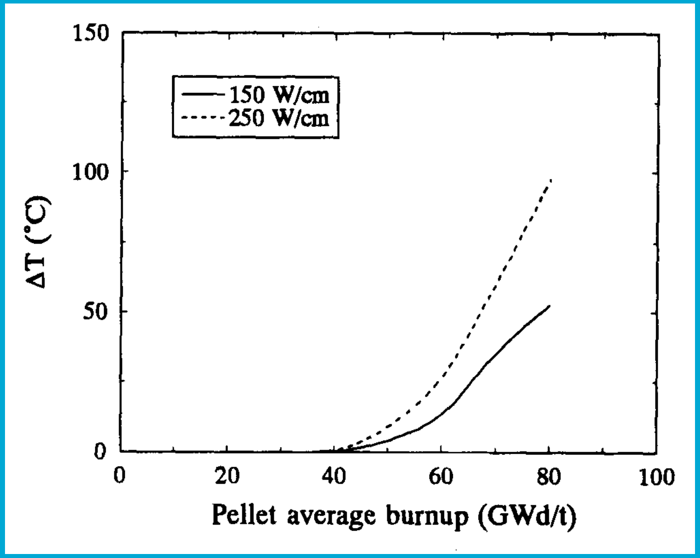
IFA-597.3 @ 60 MWd/kgUO$_2$

Measured concentration, Xe



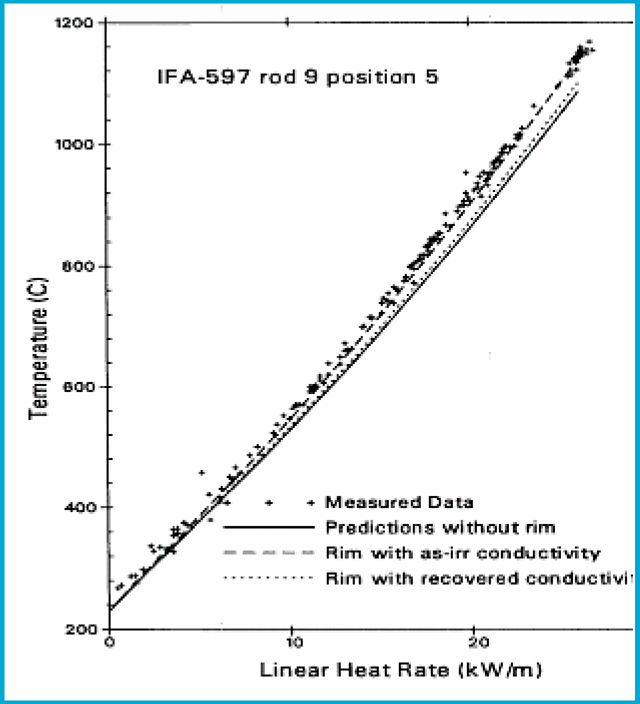
5 Conduction through pellet

…….effect of rim



Predictions by Une et al.

Comparison of predictions with experiment

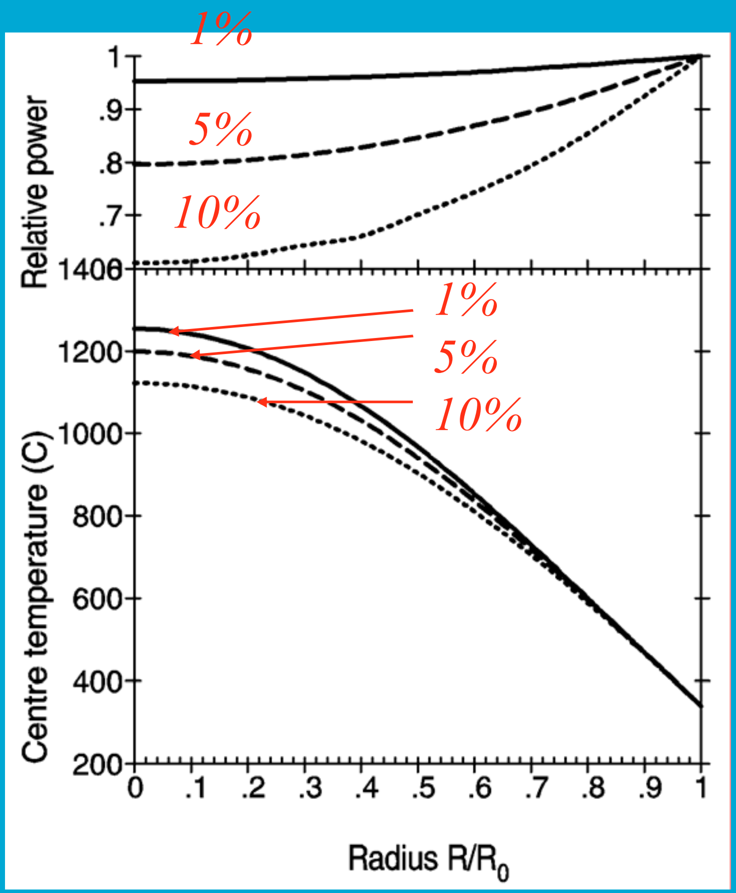


Final thoughts

…….heat generation

Self shielding at high enrichment causes more heat to be generated in outer regions of the pellet, hence lower centre temperatures for the same rating

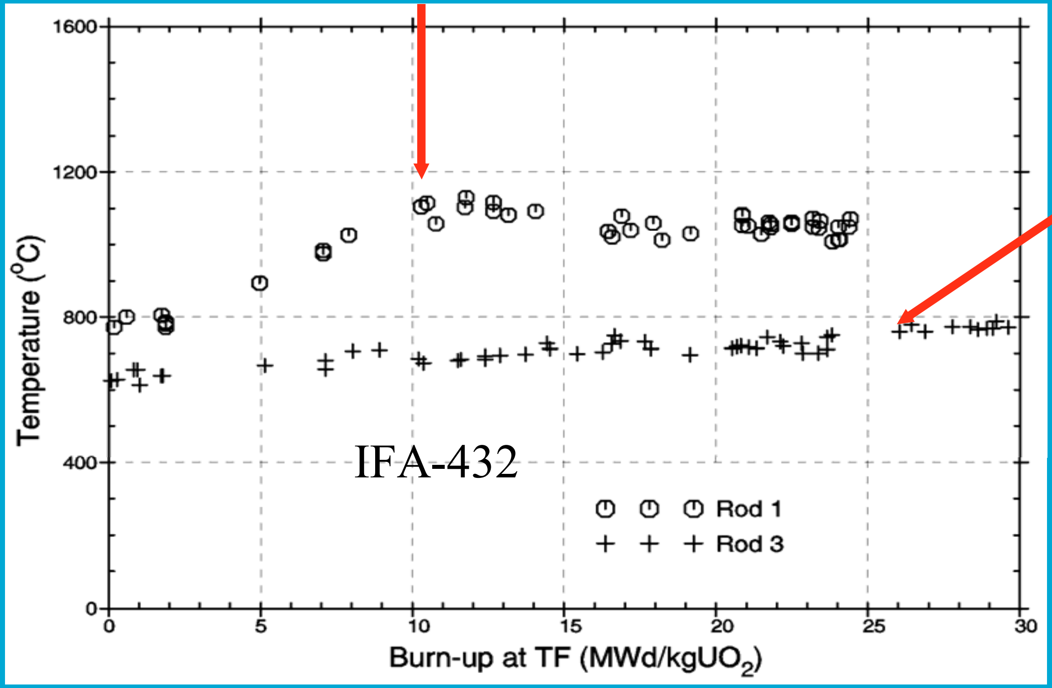
This has implications at high burn-up because of Pu generation in rim



Final thoughts

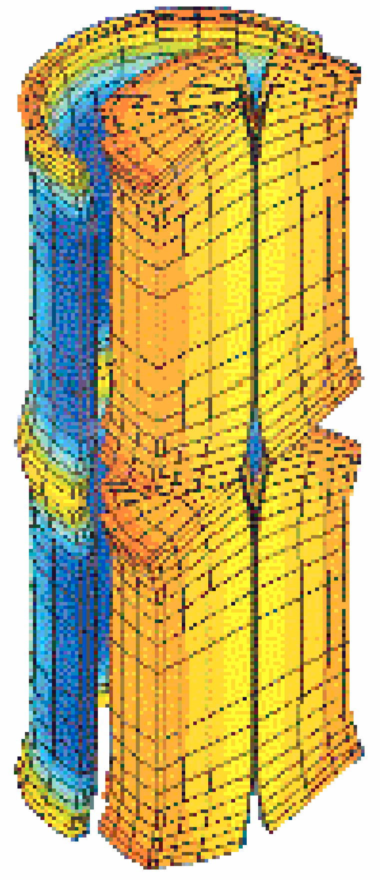
…….thermal feedback

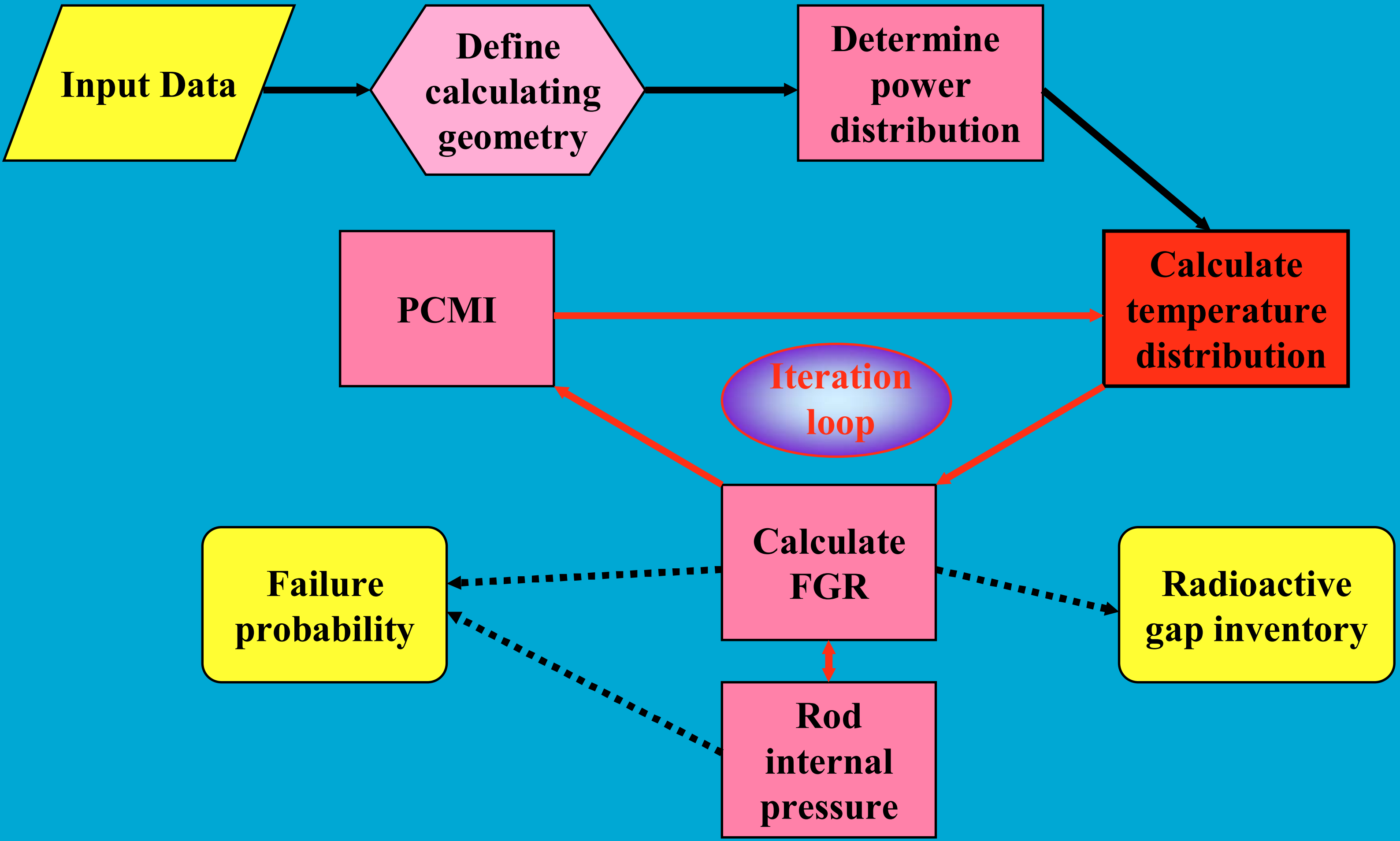
Large gap rod
thermal feedback from
released fission gas



Small gap rod
thermal conductivity
degraded with burn-up

Typical code structure





Input Data

Define calculating geometry

Determine power distribution

Calculate temperature distribution

PCMI

Iteration loop

Calculate FGR

Failure probability

Radioactive gap inventory

Rod internal pressure