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**Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for
Characterization and Basic Understanding of Radiation Damage
Mechanisms in Materials**

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**Fuel temperature modeling and phenomena:
pellet-clad gap heat transfer, fuel temperature distribution**

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Fuel Temperature Modelling and Phenomena (II)

- fuel temperature distribution -

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

Trieste, April 12-23, 2010

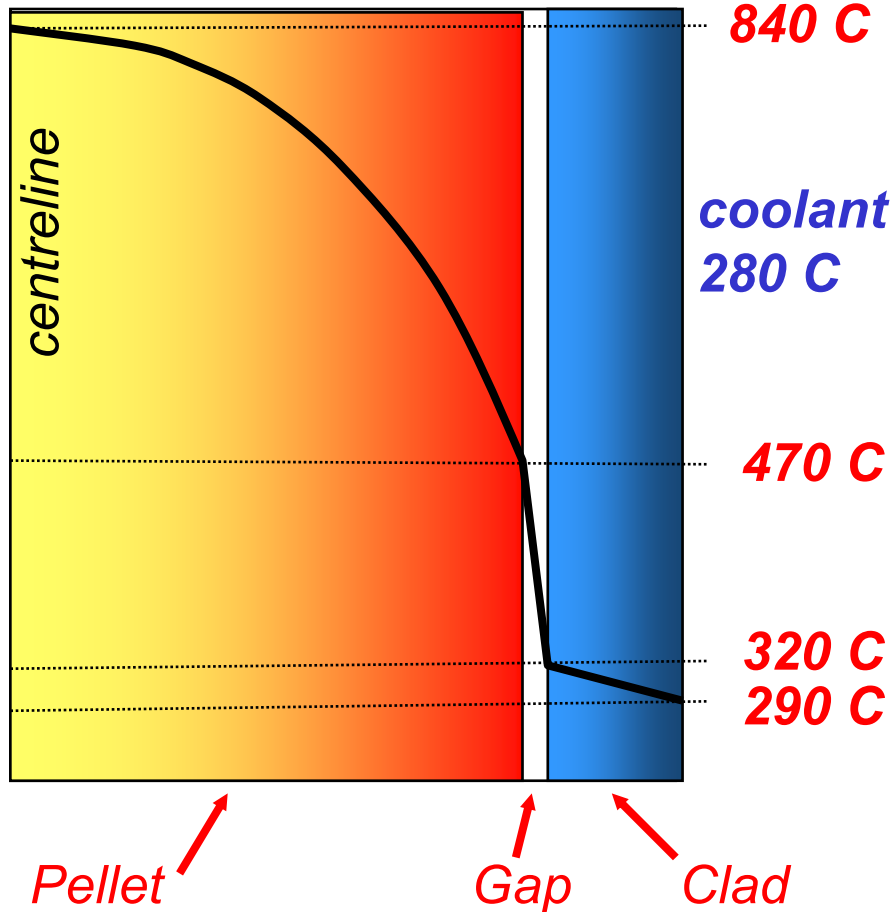
Overview

- Why temperature calculation?
- Coolant and cladding heat transfer
- Conductance through pellet-clad gap
 - open gap, gas conduction
 - closed gap, contact conductance
 - geometrical changes influencing gap size
- **Fuel temperature distribution**
 - principal formulation
 - fuel conductivity
 - power distribution



Typical temperature distribution

(20 kW/m)



Heat flow resistances

1. coolant – cladding
2. oxide/crud layer
3. cladding wall
4. inner oxidation / bonding layer
5. fuel – cladding gap
 - numerous influences
6. fuel
 - conductivity
 - general porosity
 - high burnup porous rim
 - cracks

6. Fuel temperature distribution

- general formulation -

<p>Heat balance</p> $P_v - \text{div } q = c_p \rho \frac{\partial T}{\partial t}$	P_v q c_p ρ T t	<p>power density</p> <p>heat flux</p> <p>heat capacity</p> <p>density</p> <p>temperature</p> <p>time</p>	W/m^3 W/m^2 $\text{J/g}\cdot\text{K}$ g/m^3 C s
<p>Heat conduction</p> $q = -\lambda \text{ grad } T$	λ	<p>conductivity</p>	$\text{W/m}\cdot\text{K}$
<p>Heat equation</p> $P_v + \text{div}(\lambda \text{ grad } T) = c_p \rho \frac{\partial T}{\partial t}$	<p><i>Valid in general for steady state and transient conditions</i></p>		



Simplified formulation

A fuel rod is a cylinder and most easily described in cylinder coordinates. Simplifications are possible:

- A fuel rod (pellet) is basically axi-symmetric

No heat flow in the circumferential direction

$$\frac{\partial T}{\partial \varphi} = 0$$

- In the axial direction

- no cooling at the ends

- stack interrupted by pellet-pellet interfaces

- much longer axially than radially

No heat flow in the axial direction

$$\frac{\partial T}{\partial z} = 0$$

- The fuel time constant, 5-10 s, is small compared to speed of most power/temperature changes

No consideration of time dependence

$$\frac{\partial T}{\partial t} = 0$$



Some useful equations and numbers

$$P_v + \frac{1}{r} \frac{d}{dr} \left(\lambda(T, r) \cdot r \frac{dT}{dr} \right) = 0$$

$$T(r) = T_R + \frac{1}{4} \frac{P_v}{\lambda} (R^2 - r^2)$$

$$T_0 = T_R + \frac{1}{4\pi R^2} \frac{q'}{\lambda} R^2$$

90 – 100 kW/m (UO₂)

≈ 30K per kW/m (UO₂)

- Simplified basic equation, radial dependence only
- Solved for $P_v = \text{const}$ and $\lambda = \text{const}$; $R = \text{pellet radius}$
The basic temperature distribution is parabolic
- Centre temp. expressed with linear heat rating q' (W/m)
The centre temperature T_0 is independent of radius R
- Power to melting (ca 2800°C)
- Centre temperature increase



... but we need some more details

1. Thermal conductivity of the fuel

- temperature dependence
- burnup dependence
- influence of additives (e.g. Gd)

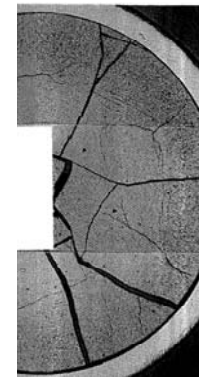
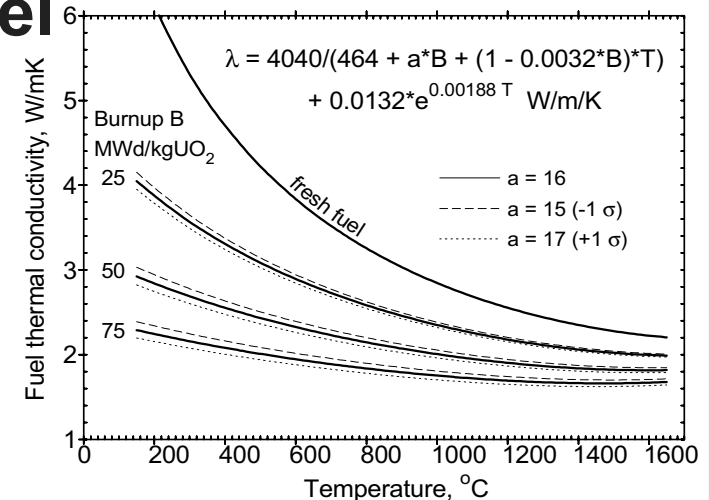
2. Influence of porosity on fuel (UO₂) conductivity

- densification (removal of pores)
- generation of new porosity by fission gas

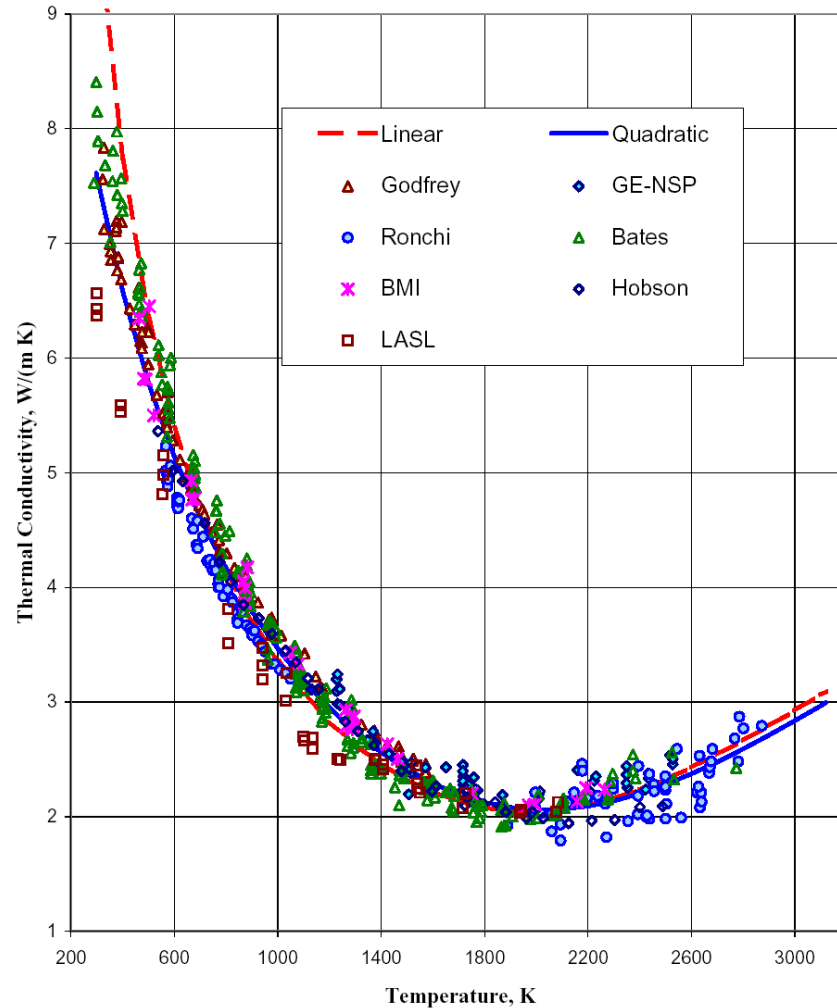
3. Influence of fuel cracking

4. Radial power distribution

- changes due to burnup and Pu generation
- burnable poisons



6.1 Thermal conductivity (UO_2)



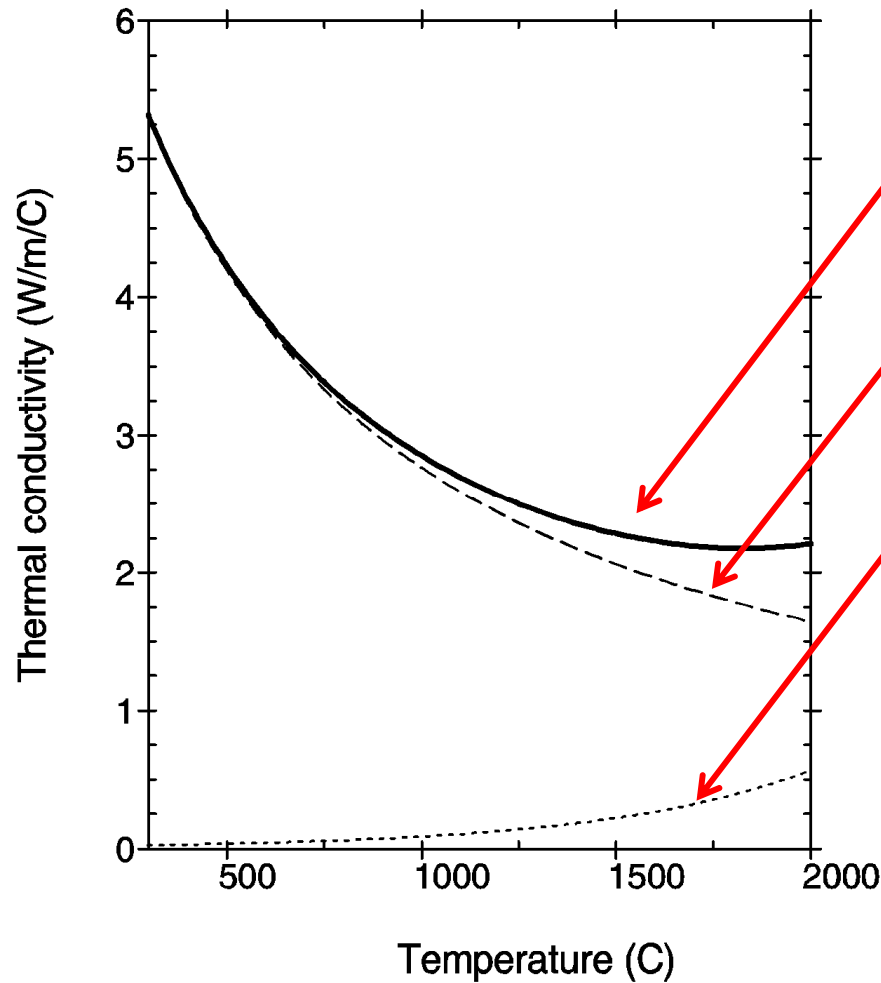
Data for UO_2
with 95%
theoretical density

UO_2 (a ceramic) is a poor heat conductor. The thermal energy is transported by lattice vibrations travelling through the lattice as waves, also known as phonons.

The data have $\pm 5\%$ spread in 600-2200K range of practical interest.



Thermal conductivity contributions



$$\lambda = \lambda_{phonon} + \lambda_{electronic}$$

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

$$\lambda_{electronic} = E_1 \cdot \exp(E_2 \cdot T)$$

In addition, λ depends on

- porosity
- burn-up
- stoichiometry



Influence of impurities

- The phonon travelling is disturbed by scattering sites
- The intrinsic scattering sites are increased by
 - additives such as Gd (burnable poison)
 - accumulation of fission products in the matrix
 - irradiation induced defects

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

$$A = A_0 + A_{Gd} + A_{bu} + A_d$$

$$A_{Gd} = c_{Gd} \cdot Gd$$

$$A_{bu} = c_{bu} \cdot bu$$

$$A_d = c_d \cdot bu$$

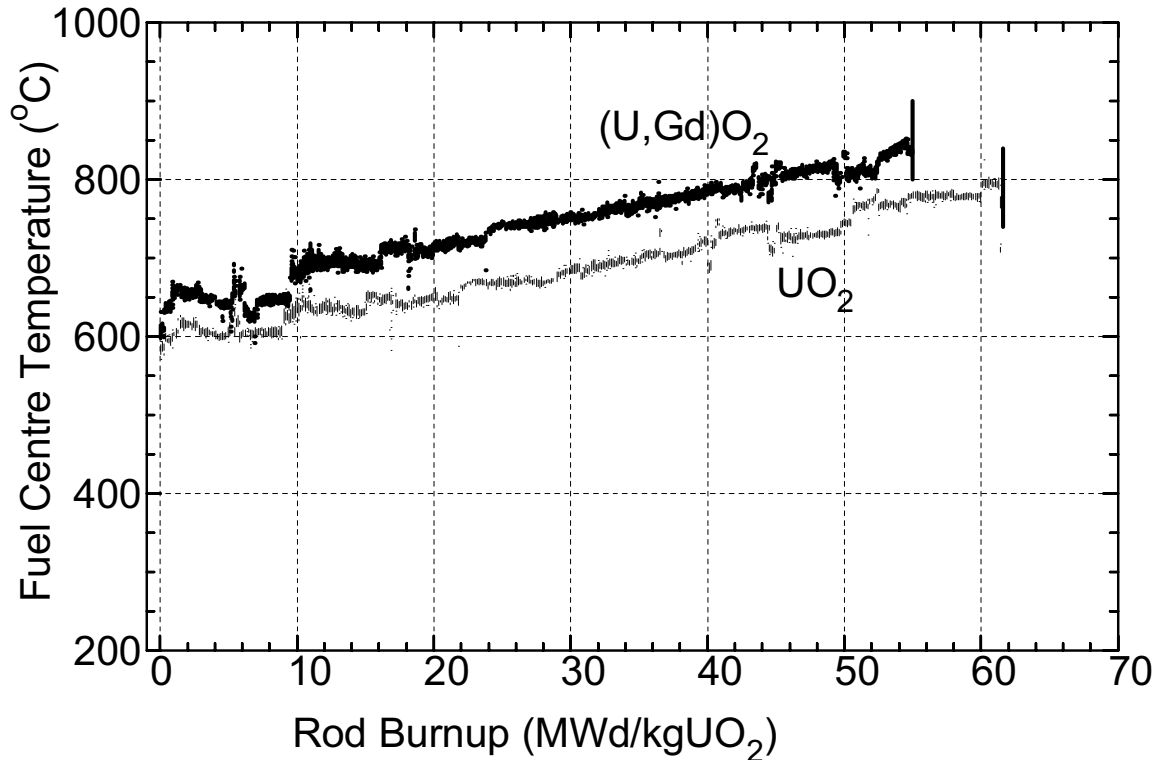
Gd = gadolinia concentr.

bu = burnup



Thermal Conductivity, Degradation

Development of temperature in UO_2 and $(\text{U,Gd})\text{O}_2$ fuel



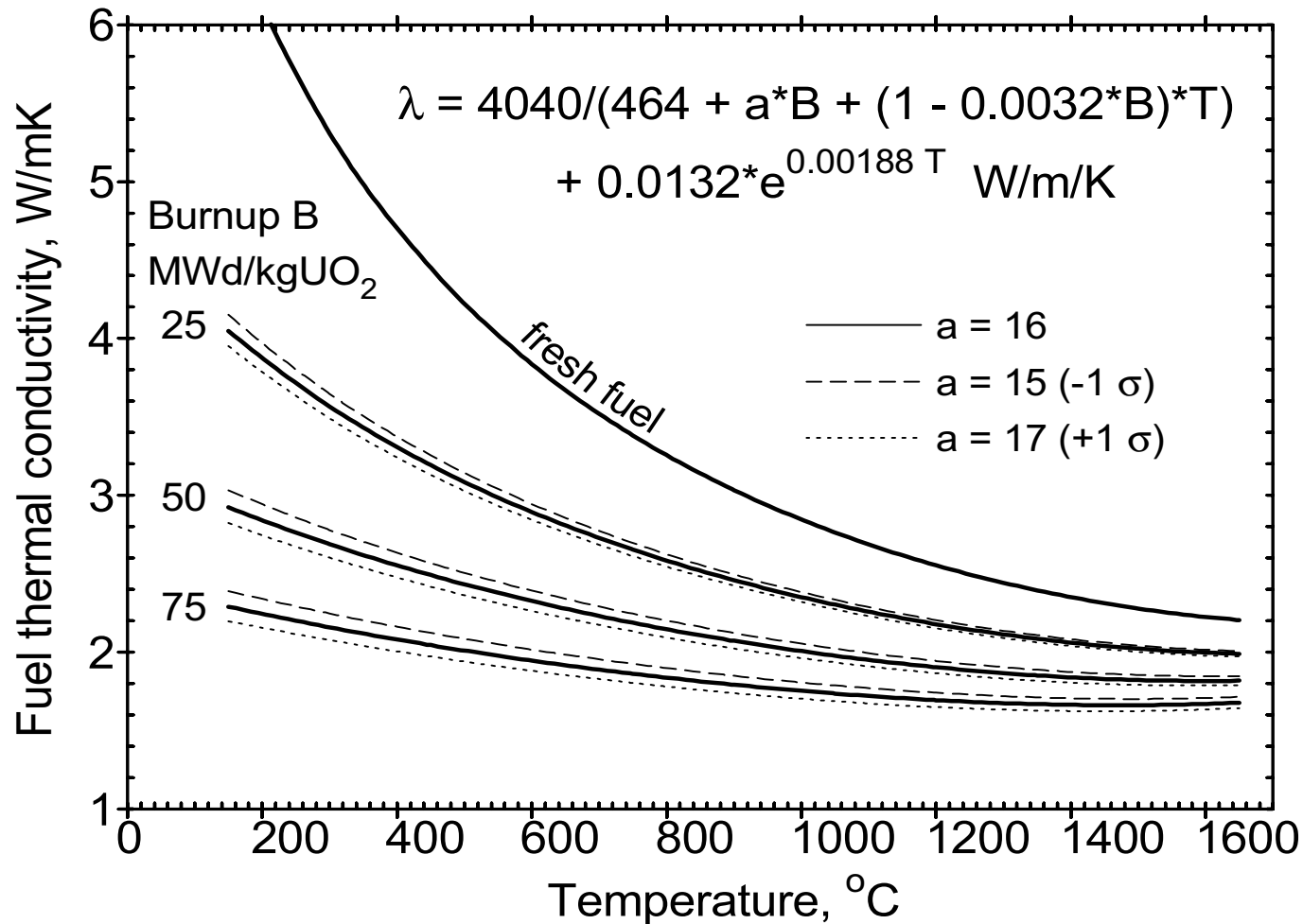
Measured fuel centre-line temperatures are linked to the thermal conductivity of the fuel.

The linear increase of the measured temperature with burnup implies a modification of the “phonon term” with a linear burnup dependent term in the denominator:

$$A_{bu} = c_{bu} \cdot bu$$

The comparative irradiation shows the conductivity difference of the two types of fuel as well as the change of conductivity with burnup.

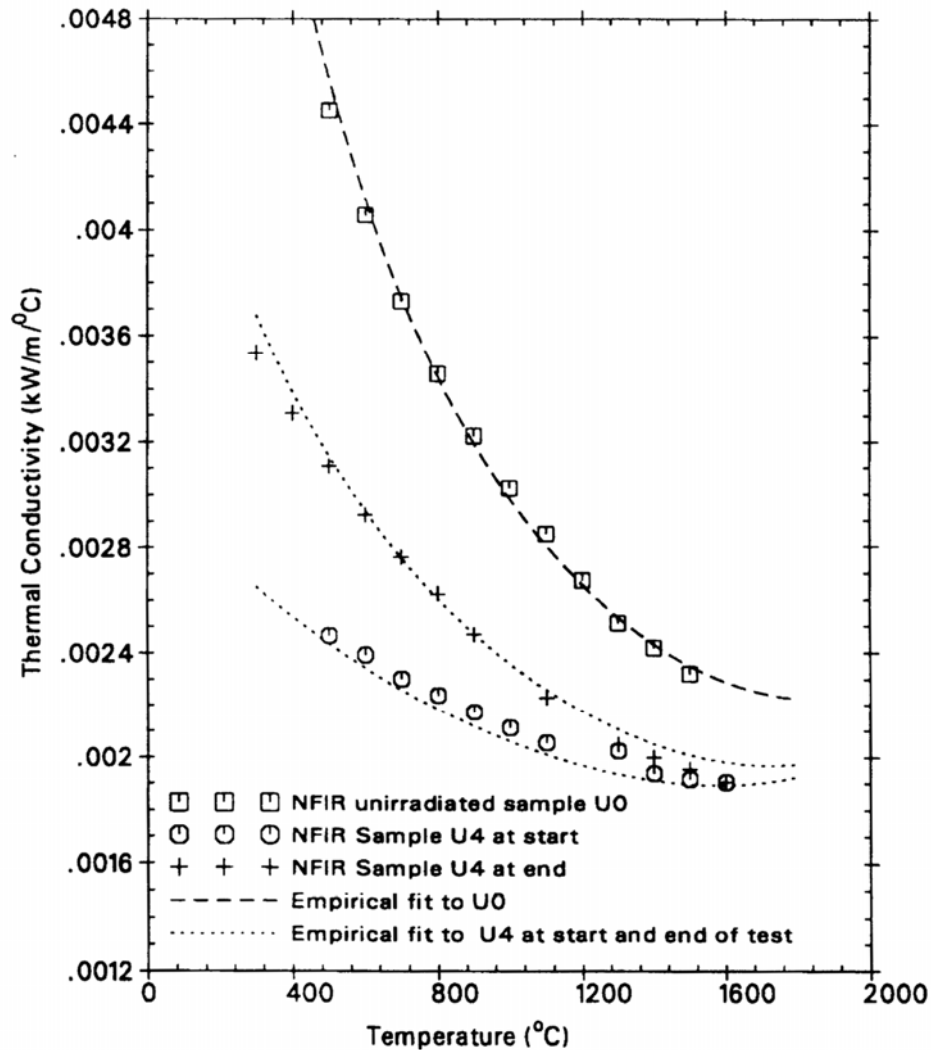




Change of UO₂ thermal conductivity derived from Halden reactor fuel temperature measurements



Laser flash conductivity measurement

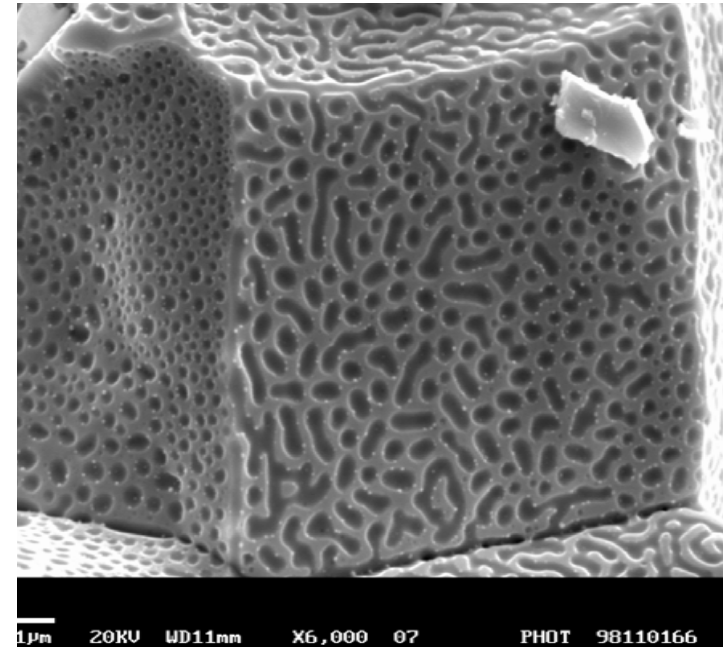


- The fuel sample is heated up to the test temperature
- The response to a laser flash can be evaluated regarding thermal conductivity
- For irradiated fuel, a marked difference between going up and down in temperature indicates annealing of phonon scattering sites
- Little is yet known about the kinetics of this effect and its dependence on in-core temperature changes



6.2 Influence of porosity on fuel (UO₂) conductivity

- Maximum achievable density by sintering is about 98% th.d. (10.96 g/cm³ for UO₂)
- Some porosity (3-5%) is desirable and achieved through adding pore formers to the powder before sintering
- The porosity changes during irradiation
 - destruction/removal of pores by fission spikes (densification)
 - formation of fission gas bubbles
 - intragranular
 - intergranular
 - on grain edges and faces



Porosity correction factors

- For fuel with porosity P , the conductivity is modified with:

$$\lambda_p = f(P) \cdot \lambda_0$$

- Various formulations for $f(P)$:

$$f = 1 - 2.5P \quad (\text{Loeb})$$

$$f = (1-P)/(1+0.5P) \quad (\text{Maxwell})$$

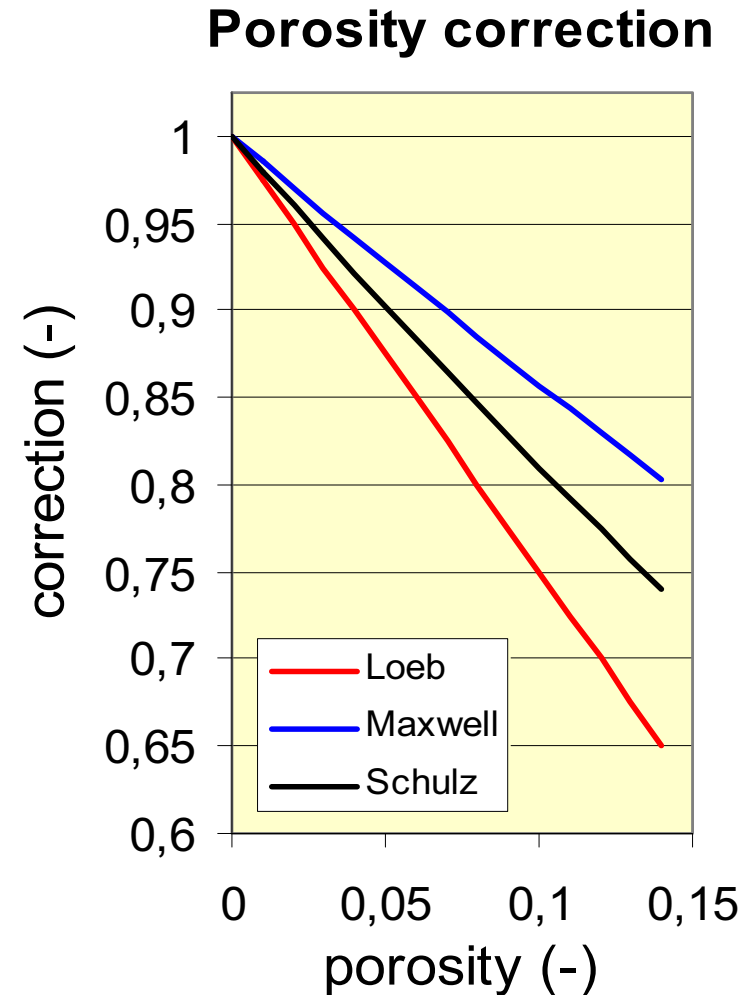
$$f = (1 - P)^2 \quad (\text{Schulz})$$

$$f = (1-P_1)(1-P_2)^{2.5}(1-P_3)^{3.5} \quad (\text{Harding})$$

P_1 = coarse spherical pores

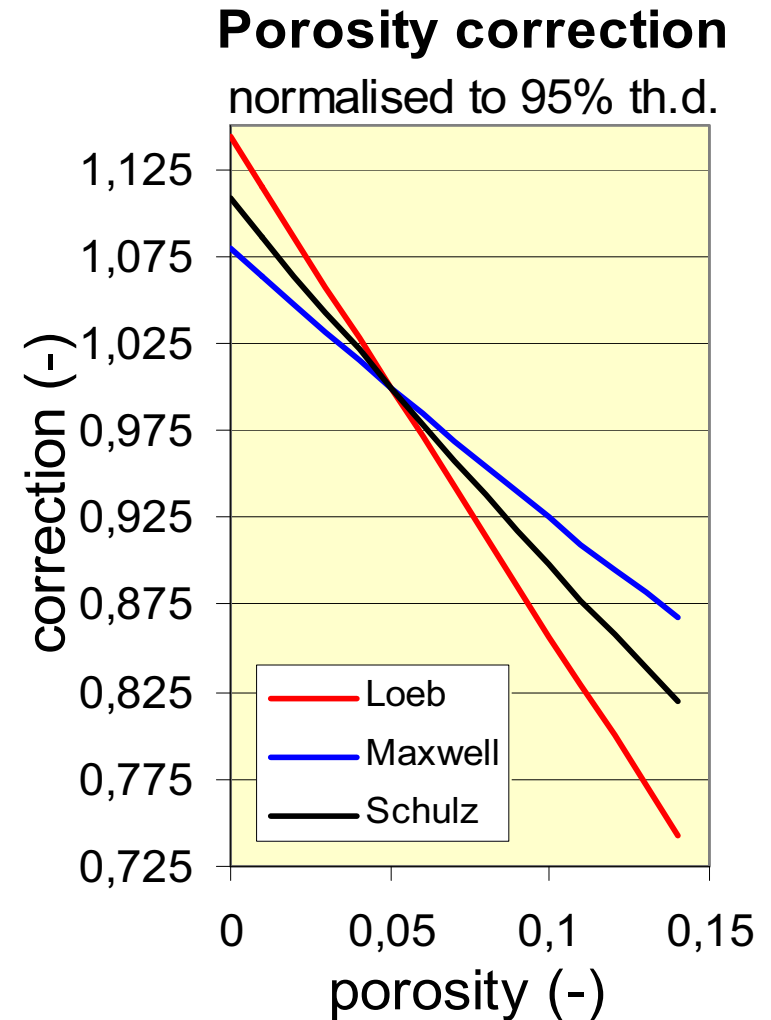
P_2 = fine spherical pores

P_3 = grain face pores



Beware!

- Conductivity is sometimes given for 100% dense fuel. This means that a certain correction was applied to the data obtained with less dense fuel (often 94-96% th.d.)
- When applying a different porosity correction, the conductivity data should also be transformed back to the original density

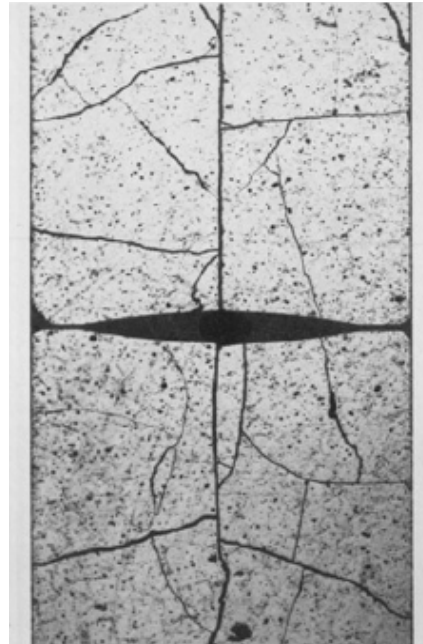
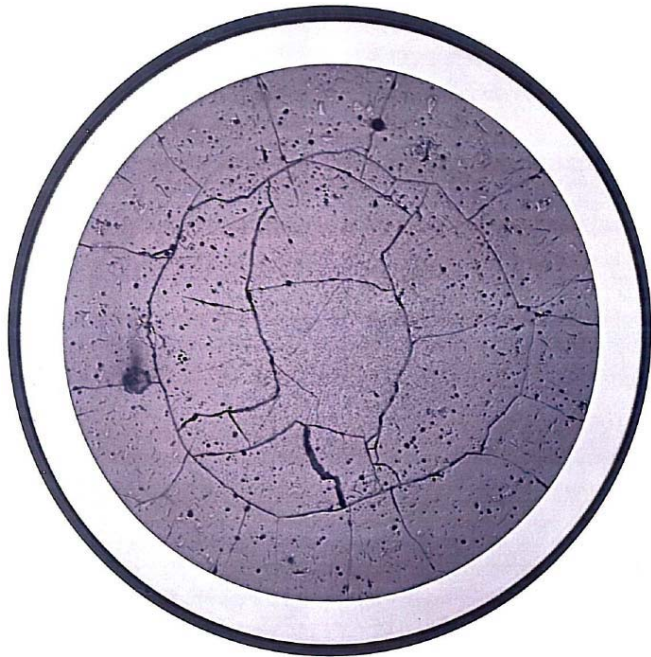


6.3 Influence of fuel cracking

- Cracking of the UO_2 fuel pellets reduces the effective fuel thermal conductivity
- This effect may be approximated by
 - appropriately chosen "crack factors" that reduce the solid- UO_2 thermal conductivity
 - introduction of cracks in the geometry and modelling of the temperature increase across the crack in a way similar to that for the fuel-cladding gap
- Circumferential cracks are most "efficient", but they only develop at cool-down after long periods at high power
- In general, the cracking pattern is not known and may even be influenced by the introduction of a TC



Examples of fuel cracking

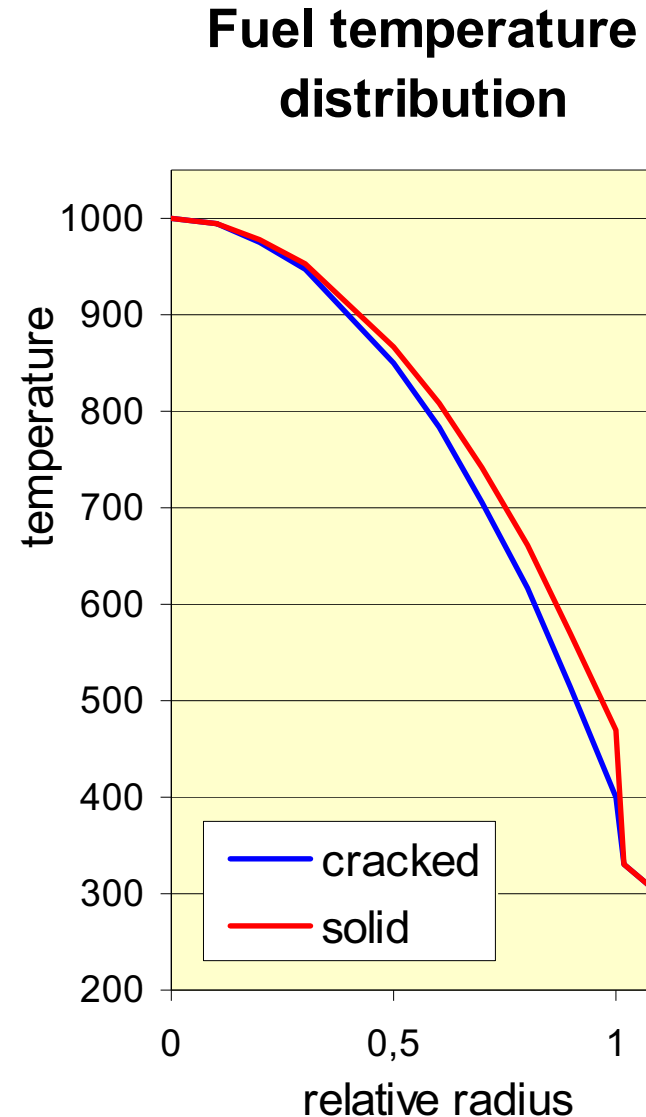


Heat flow resistances are introduced by

- circumferential cracks
- cracks deviating from the radial direction
- transversal cracks deviating from the plane normal to the axial direction

Consequences

- The temperature calculation in fuel modelling codes is linked to measured fuel centre temperature data
- Since a codes must stay tuned to the data base, the assumption of reduced fuel conductivity results in a reduction of the fuel stored energy, regardless of the modelling approach
- Accounting for fuel cracking leads to lower calculated peak clad temperatures obtained in some loss-of-coolant accident simulations

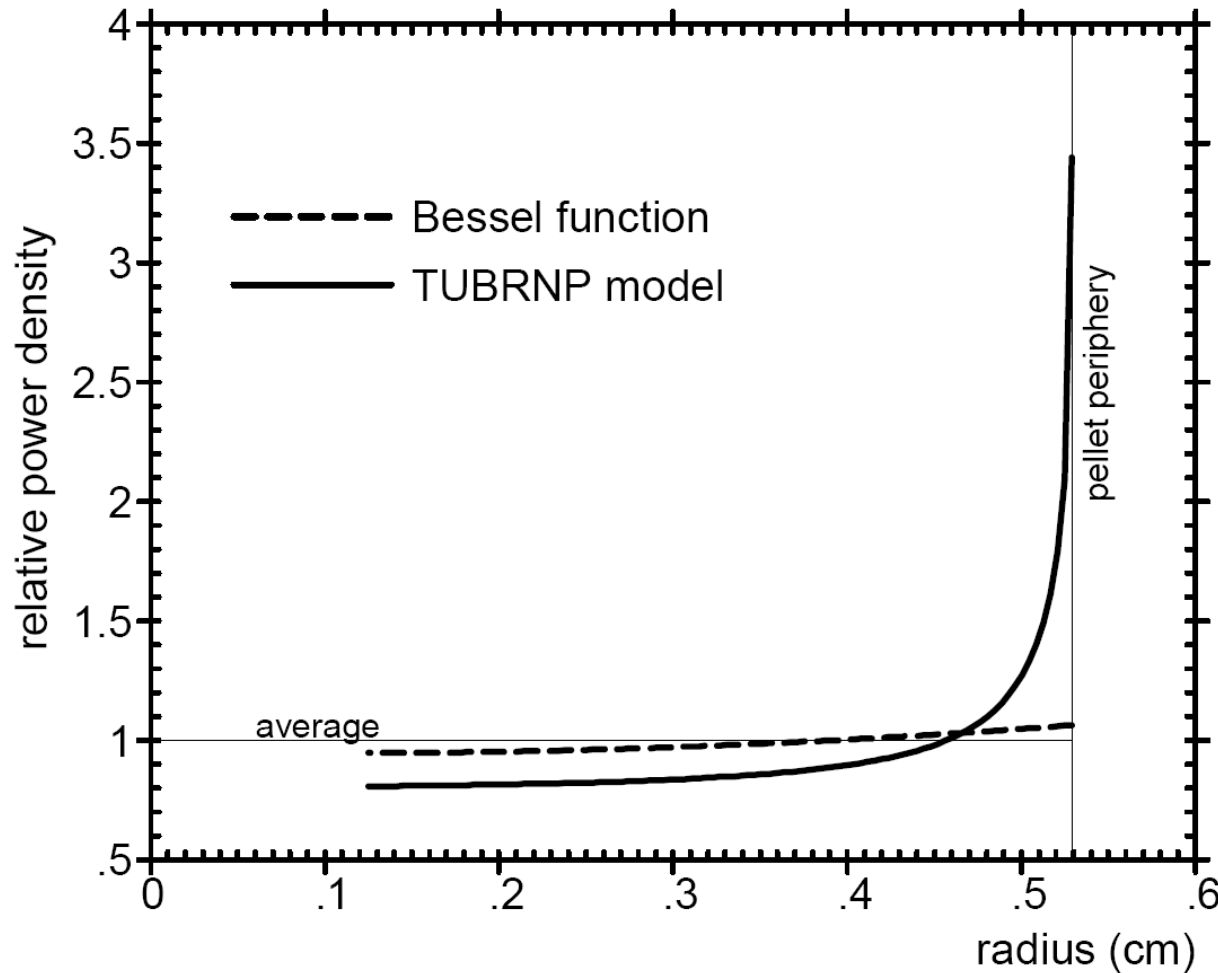


6.4 Radial power distribution

- Thermal neutrons are absorbed in the fuel (mostly causing fission)
- These neutrons are not replaced locally (fission neutrons have high energies)
- The net result is a neutron flux depression that depends on geometry (radius) and enrichment
- Over time, Pu will build up in the pellet periphery due to U-238 neutron absorption resonances in the epithermal energy region, resulting in a strongly edge-peaked radial power distribution



Power distribution in high burnup fuel

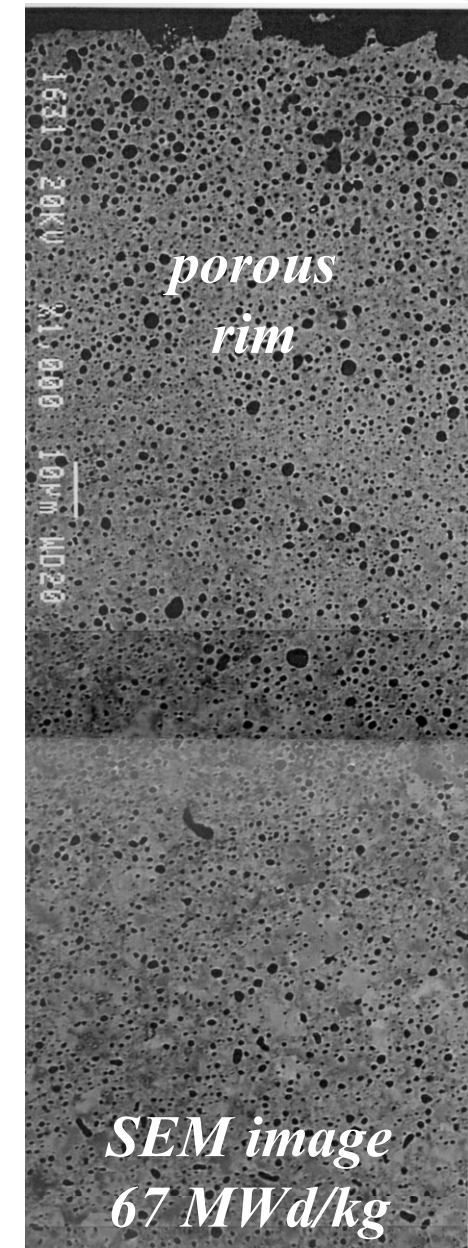


- The TUBRNP model was developed to calculate the radial power and burnup distribution, taking into account the Pu build-up.
- Alternatively, more sophisticated lattice codes can be used, but differences are small.



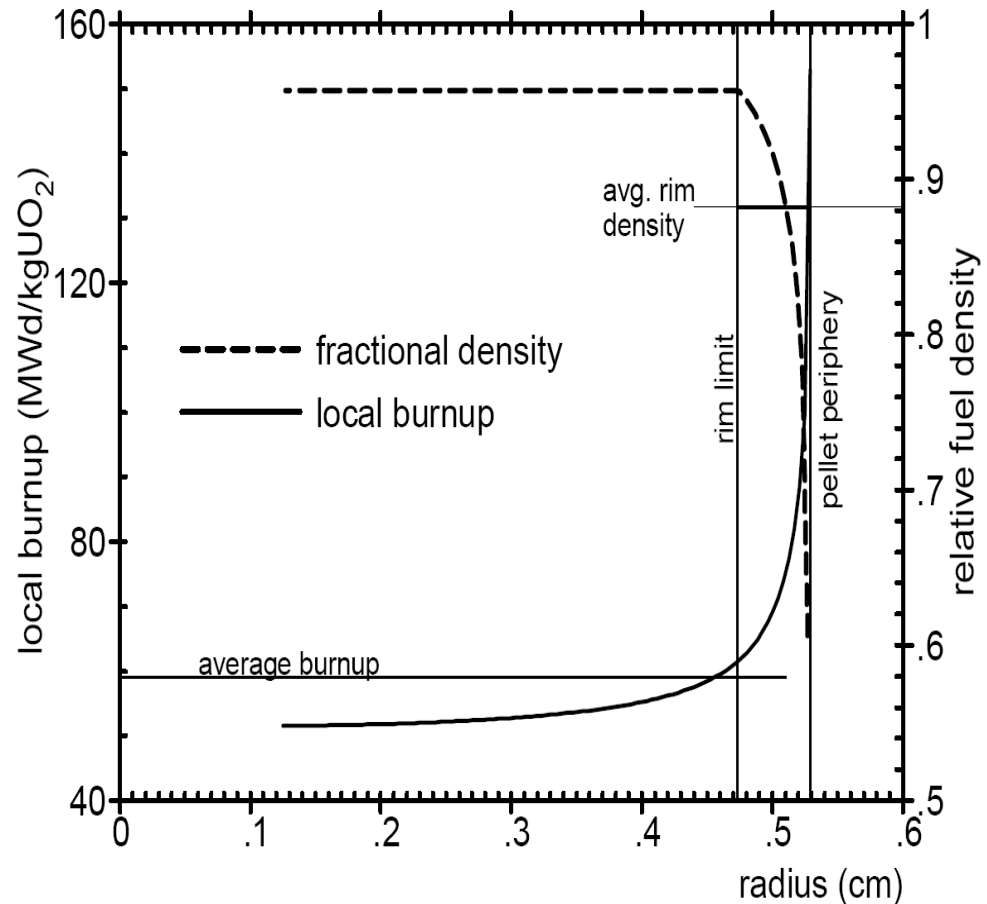
Burnup distribution and rim structure

- The periphery-peaked power generation causes a similar burnup distribution and the formation of the so-called *rim structure*
 - as fabricated grains subdivide into very small grains ($<0.1\mu\text{m}$)
 - generation of spherical pores containing fission gas at high pressure
- The fuel shown to the right has undergone considerable changes:
 - loss of defined grains up to $100\ \mu\text{m}$ into the fuel
 - development of spherical porosity reaching about $500\ \mu\text{m}$ into the fuel
 - bonding layer between fuel and cladding
- The conductivity of rim material is presently being determined (laser flash method)



Estimation of rim porosity

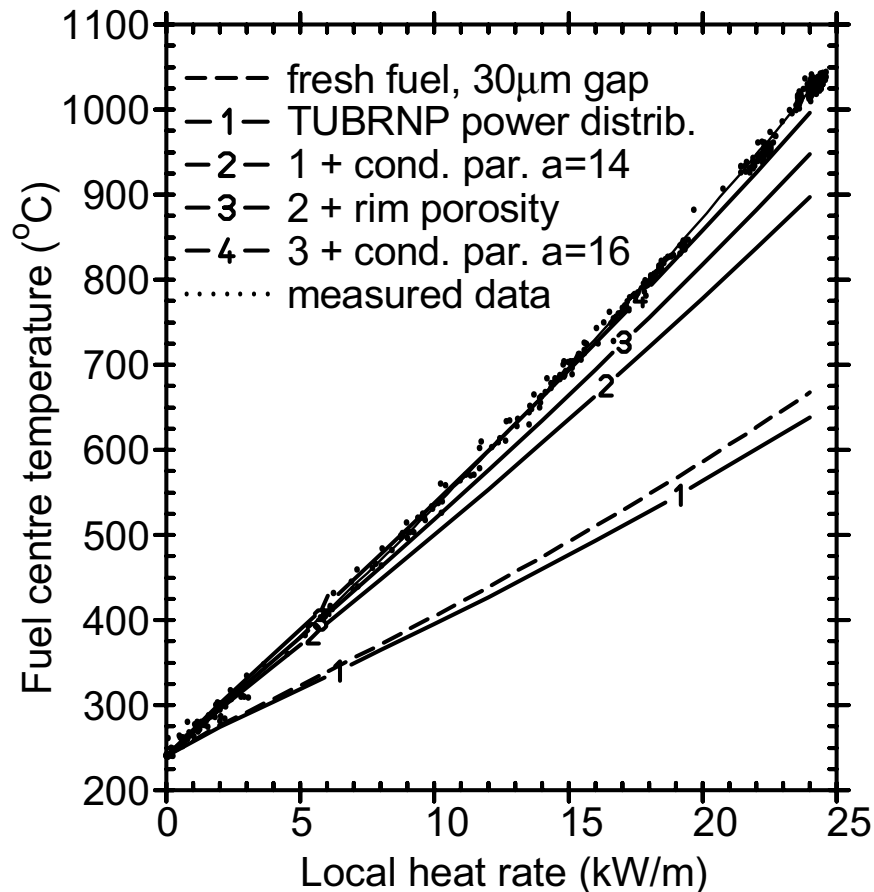
- Extra porosity is produced when the local burnup exceeds 70 MWd/kgU (full rim structure formation)
- The porosity increases linearly with burnup in excess of rim formation burnup
- 0.5% extra porosity is generated per 1 MWd/kgU beyond rim formation burnup



Burnup distribution calculated
with the TUBRNP model



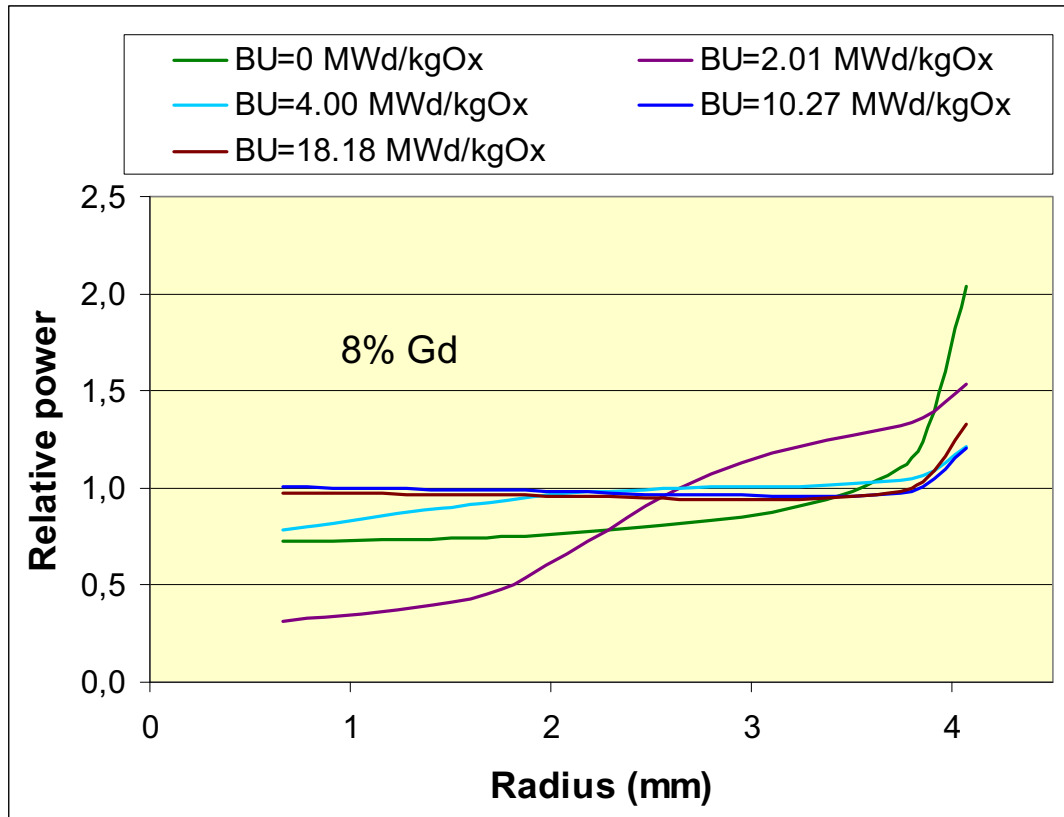
Thermal behaviour of high burnup fuel - combined effects -



- 67 MWd/kg fuel reinstrumented with fuel thermocouple
- Appreciable difference to temperatures of fresh fuel
- Important factors:
 - conductivity degradation
 - power distribution
 - rim porosity
- The model for UO_2 conductivity degradation derived from in-core temperature data is suitable for explaining the differences



Power distribution in fuel with burnable poison (Gd)



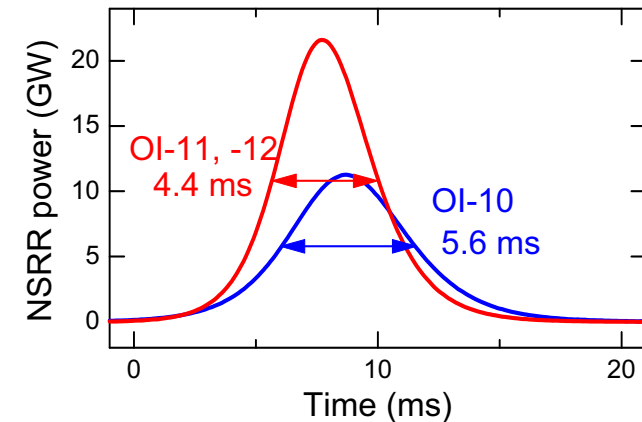
Helios calculated radial power distribution in Gd-bearing fuel (Halden IFA 681)

- The evolution of the radial power distribution in fuels with burnable poison is a complicated function of neutron fluence and spectrum
- Fuel modelling codes would take such distributions as input



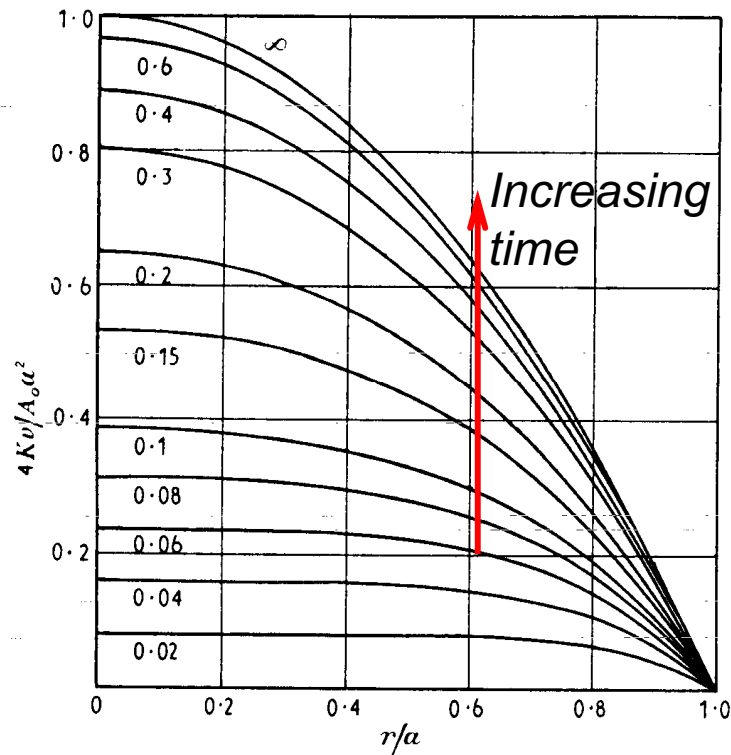
Time dependent temperature distribution

- Required for fast power changes
 - reactivity insertion accidents (RIA)
 - BWR power oscillation
 - reactor scrams
 - (loss-of-coolant accident)
- Many fuel modelling codes do not treat non-steady state temperatures
- Some divide the problem into steady state and transient treatment (e.g. Frapcon/Fraptran)
- Some implement rigorous solutions
 - Enigma, Transuranus ...
 - For proper rendering of measured data, the thermocouple response should be included in the solution



Time dependent temperature distribution

(for temperature independent conductivity and constant heat gen.)



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

Solution:

diffusivity

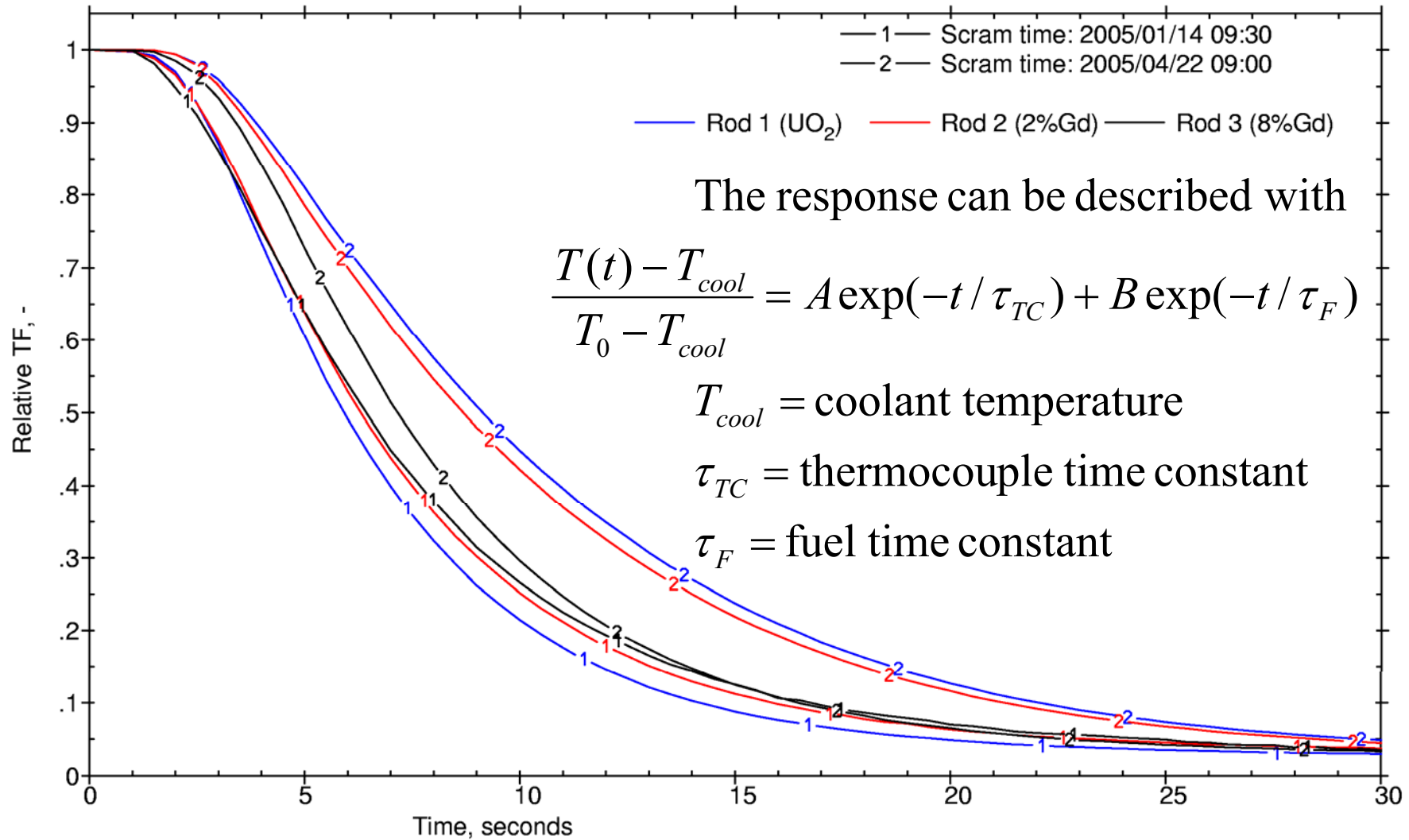
Bessel functions

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

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



Temperature response to reactor scram



Properties of the fuel time constant

- The simplified time dependent solution identifies the basic influences of geometry and material parameters on the major fuel time constant
- Changes over time occur due to
 - conductivity degradation (λ)
 - fission gas release (h)

$$\tau = \frac{R^2 \cdot \rho \cdot c_p}{\lambda \cdot a_1^2}$$

R = pellet radius

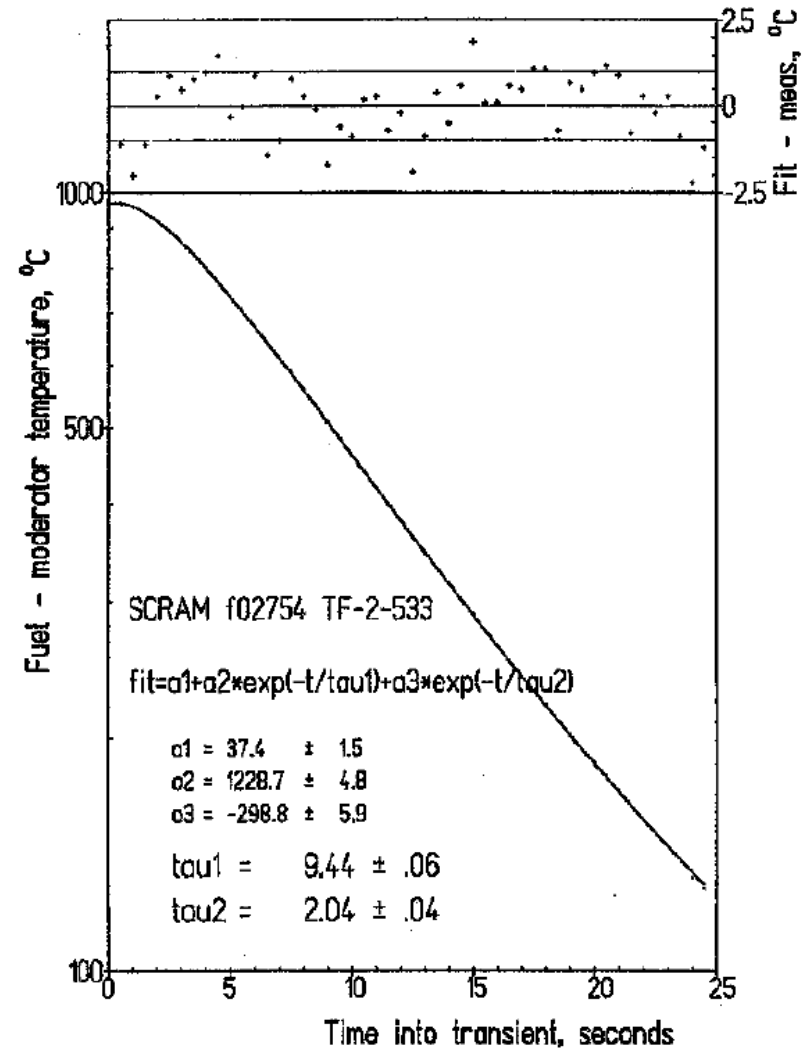
$$a_1 = h \frac{R J_0(a_1)}{\lambda J_1(a_1)}$$

J_0, J_1 = Bessel functions



Application to real data

- A scram of the Halden reactor triggers a fast data logging system which saves all temperature data every 0.5s
- The function coefficients (e.g. time constants) are determined with a least squares fitting procedure
- These data, when collected over longer periods, provide supplementary information on
 - fuel conductivity changes
 - fission gas release (gap cond.)



Typical time constants

- The *thermocouple time constant* represents a delayed registration of the actual fuel temperature
 - typical values are 0.5 – 2.0 s
 - values depend on the thickness of the TC (mass) and the heat transfer from the TC to the fuel (fuel – TC gap)
- The *major fuel time constant* depends on geometry and heat transfer properties
 - values range from 3s (small diameter fuel, $R < 3\text{mm}$) to about 10s (test rods filled with Xe)
 - typical values for standard geometry are 4 – 8s
 - Temperatures associated with power changes occurring over minutes or longer can be treated with steady state calculation
- Evaluation by noise analysis results in similar values; differences reflect response at different locations (centre, periphery, fuel average)



Summary – fuel temperatures

- Fuel temperatures and their development with burnup are influenced by many phenomena which interact in complicated ways
- First principal models as well as empirical data and correlations are employed in solving the problem
- The Halden reactor experimental data constitute a solid basis for model development and verification
- However, due to the nature of the problem, knowledge on many details will be deficient or lacking, and considerable uncertainties associated with fuel temperature calculations must be expected





The END

