REDUCTION OF RADIOLOGICAL ACCIDENT CONSEQUENCES

Title	# Fuel behaviour tools
Speaker:	Paul VAN UFFELEN
Affiliation:	European Commission, DG Joint Research Centre, Karlsruhe
Event:	R2CA Summer School
When:	4-6 July 2023
Where:	ENEA Bologna

This project has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 847656.

Importance

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Ensure safe and economic operation of fuel rods

  → predict their behaviour and life-time

- Description of fuel rod's behaviour involves various disciplines
  - Chemistry
  - Nuclear and solid state physics
  - Metallurgy and ceramics
  - Applied mechanics

  } Strongly interrelated

→ Development of fuel performance codes

General outline

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

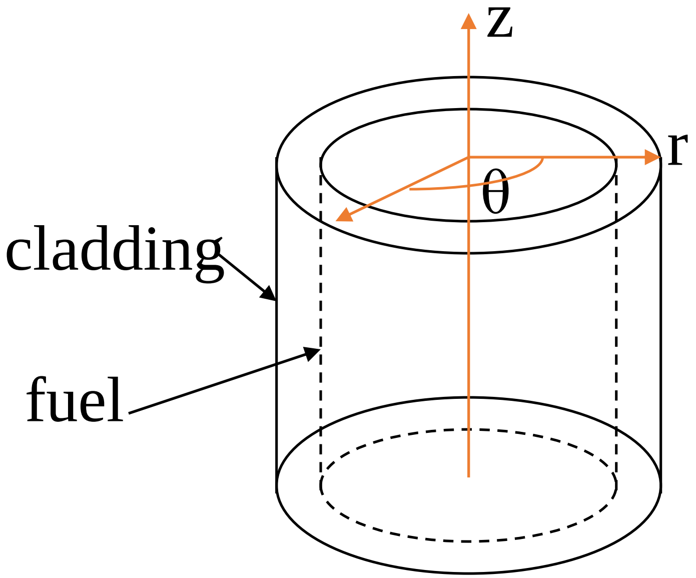
- Basic equations and limitations
  - Heat transfer
  - Mechanical analysis
  - Fission gas behaviour
- Coupling of modelling / experimental data

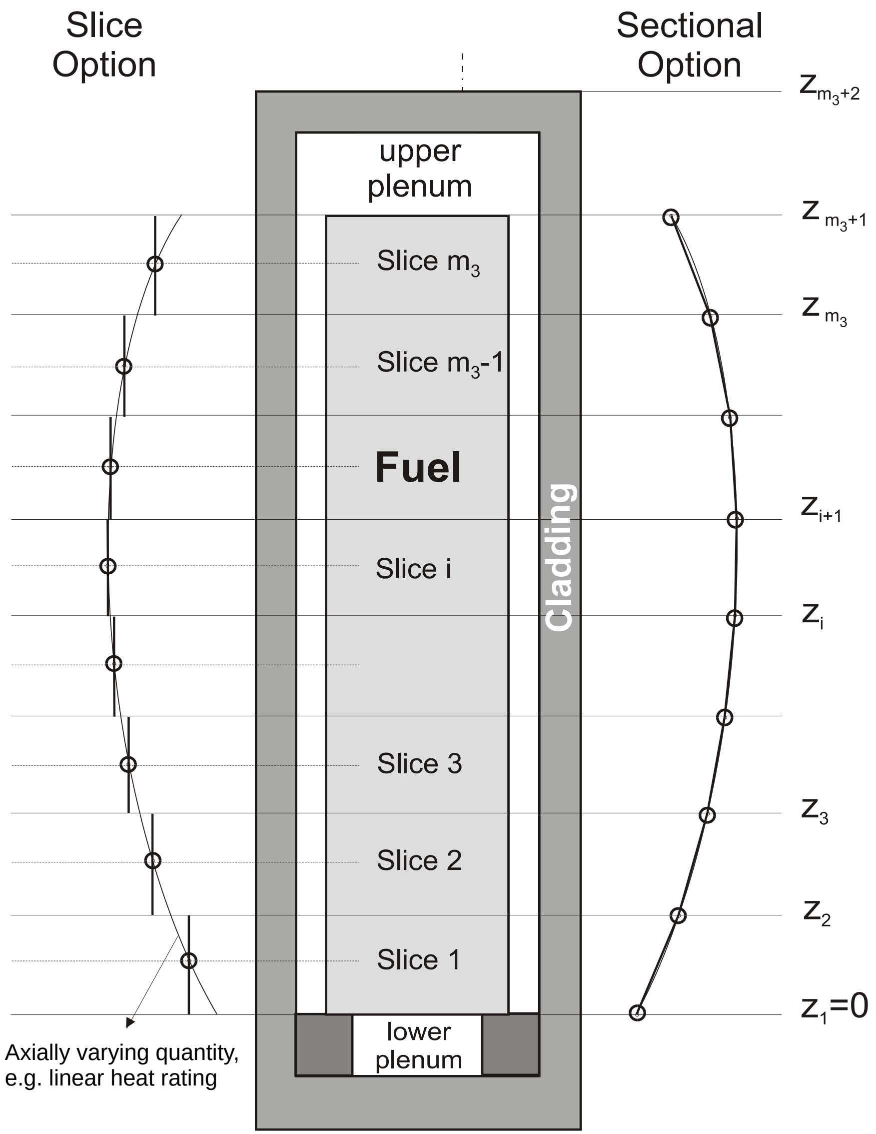
General assumptions

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

1. Fuel element with cylindrical geometry
2. Axisymmetric revolution of the rod
3. Radial T-gradient >> axial T-gradient

→"1.5 D"





Heat transfer

REDUCTION OF RADIOLOGICAL CONSEQUENCES
OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

1. In the coolant
2. Through the cladding
3. In the fuel-to-clad gap
4. In the pellets
5. The structure of the thermal analysis

Heat flow in fuel-cladding gap
Three parallel conduction routes

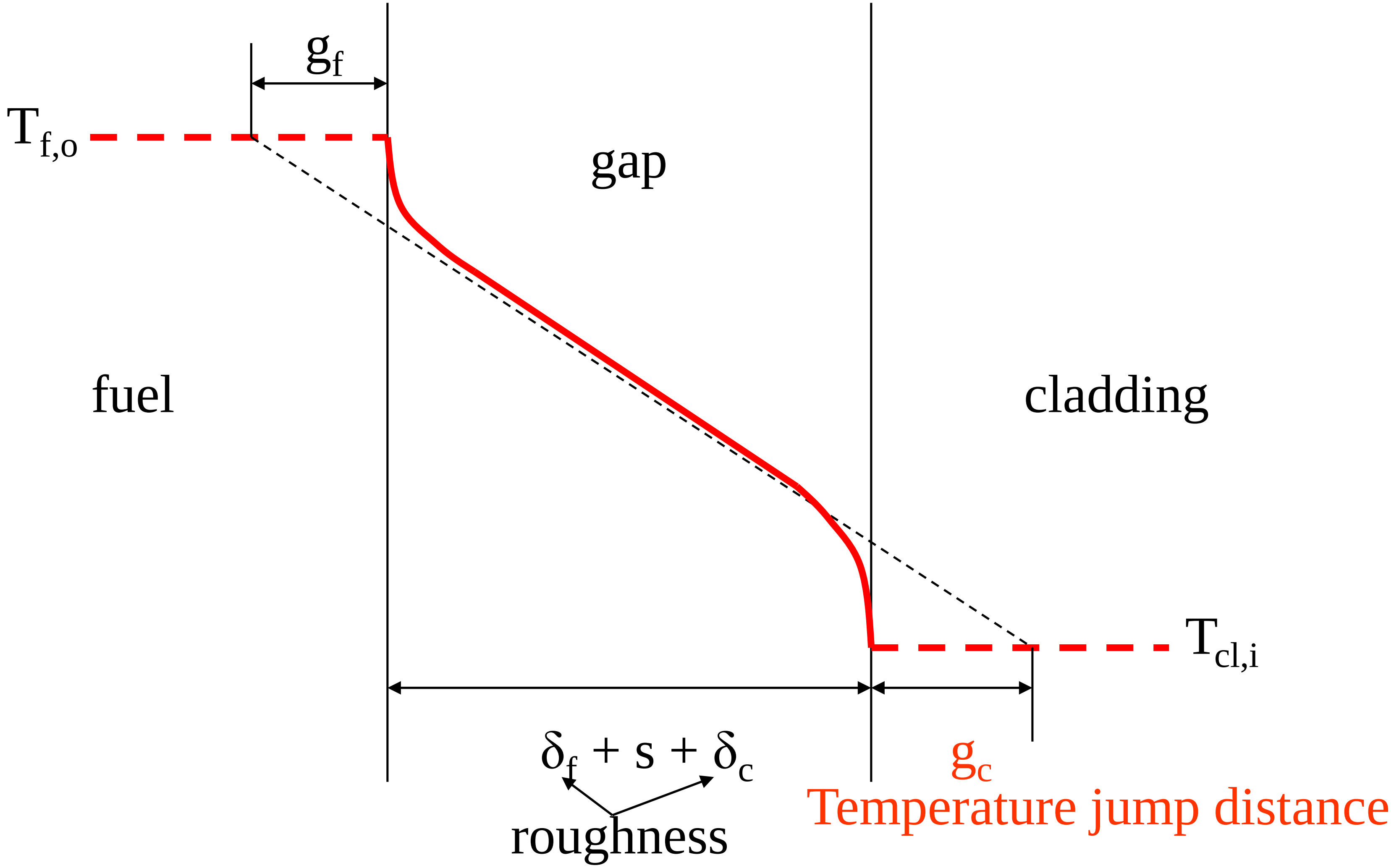
$$\Delta T_{gap} = \frac{q''}{h_{gap}}$$

$$h_{gap} = h_{rad} + h_{con} + h_{gas}$$

$$h_{gas} = \frac{\lambda_{gas}}{\delta + s + g_f + g_{cl}}$$

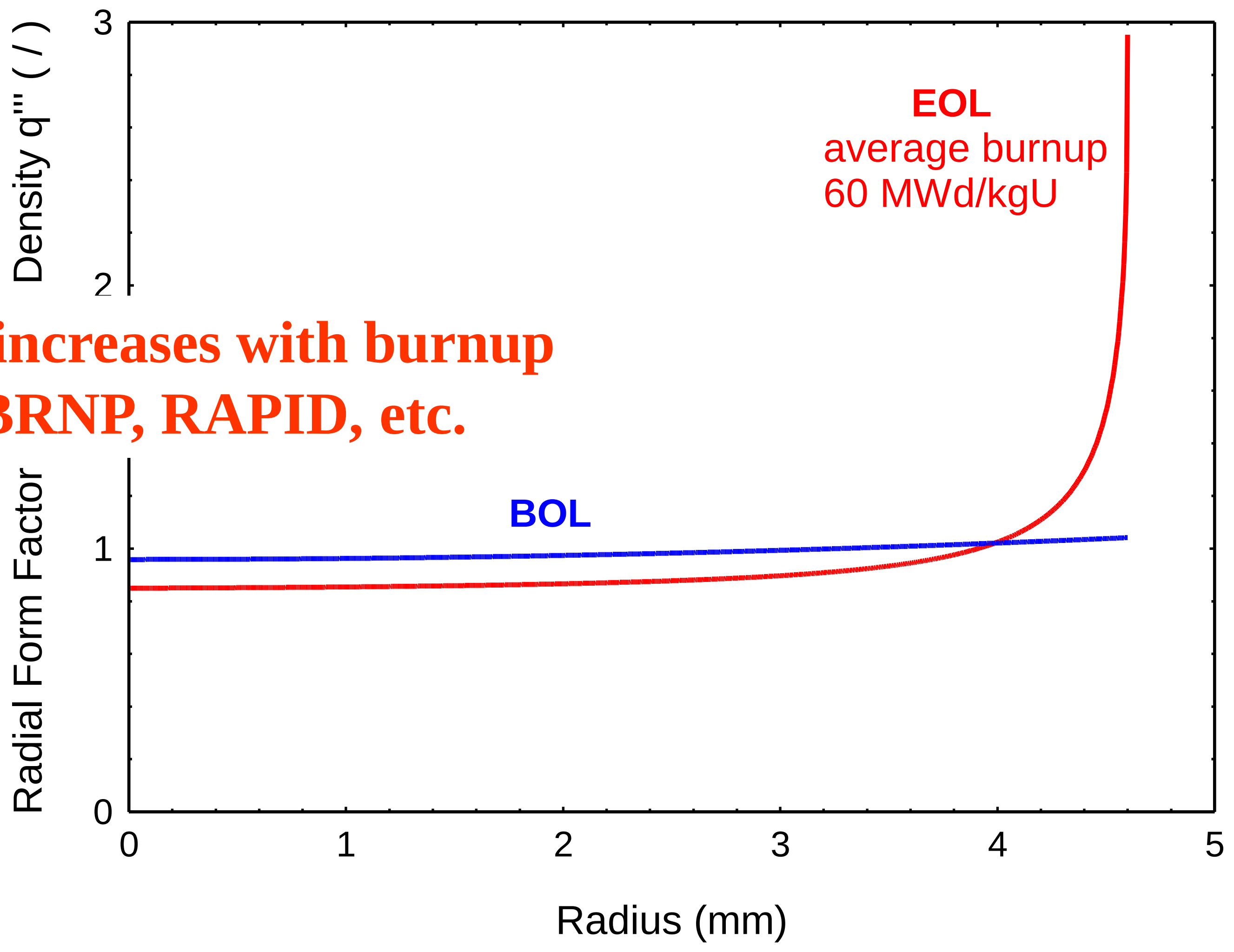
uncertainty

Schematic T profile through the gap



Heat flow in the fuel pellets
The source term

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



Gradient increases with burnup
→TUBRNP, RAPID, etc.

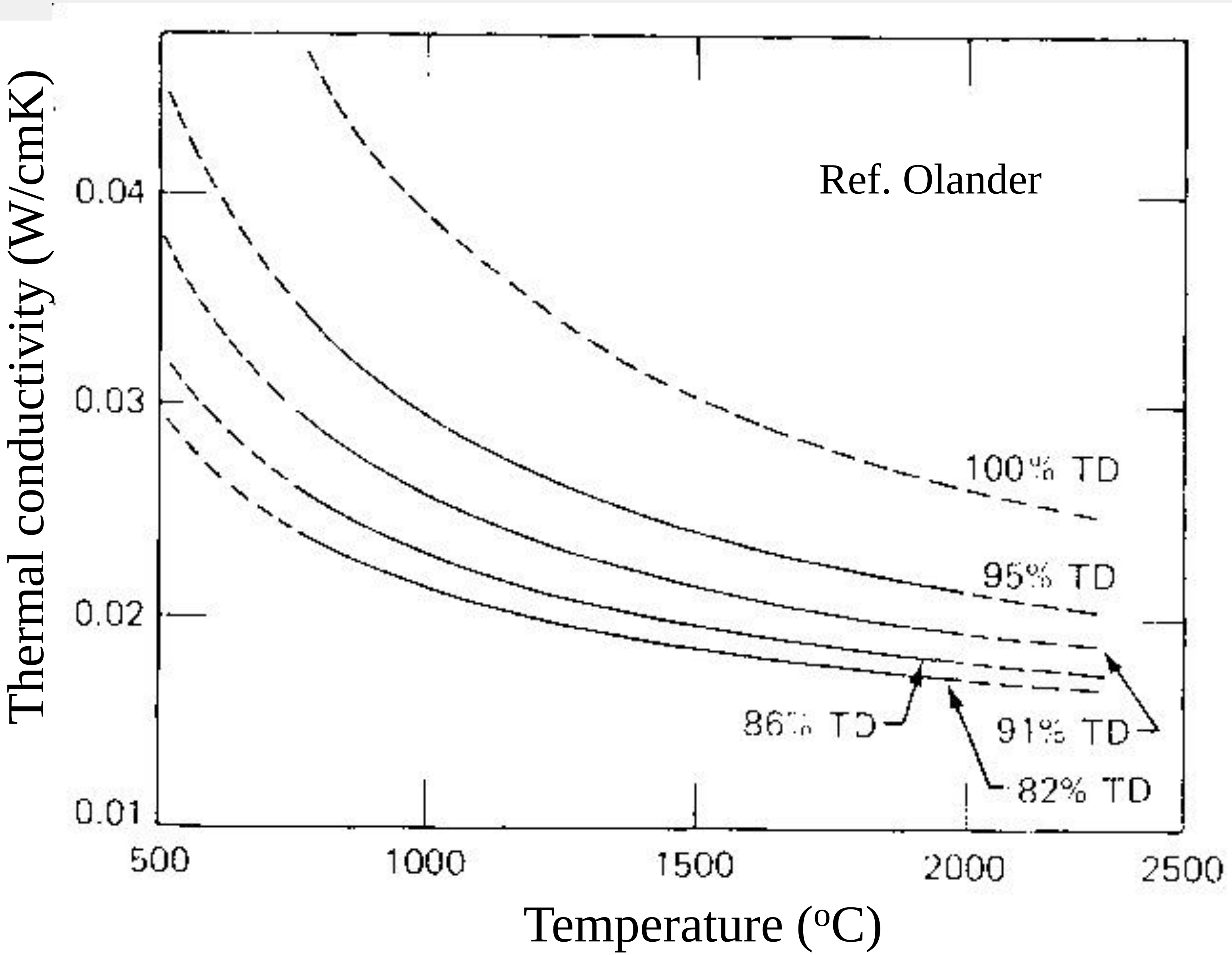
Fuel thermal conductivity
Effect of various parameters

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Density (pore size, shape, orientation)
  - Loeb (modified) $$\lambda = \lambda_{100\%}\left(1-\alpha P\right)$$
  - Maxwell-Eucken $$\lambda = \lambda_{100\%}\frac{1-P}{1+\alpha P}$$
- Composition
- Irradiation

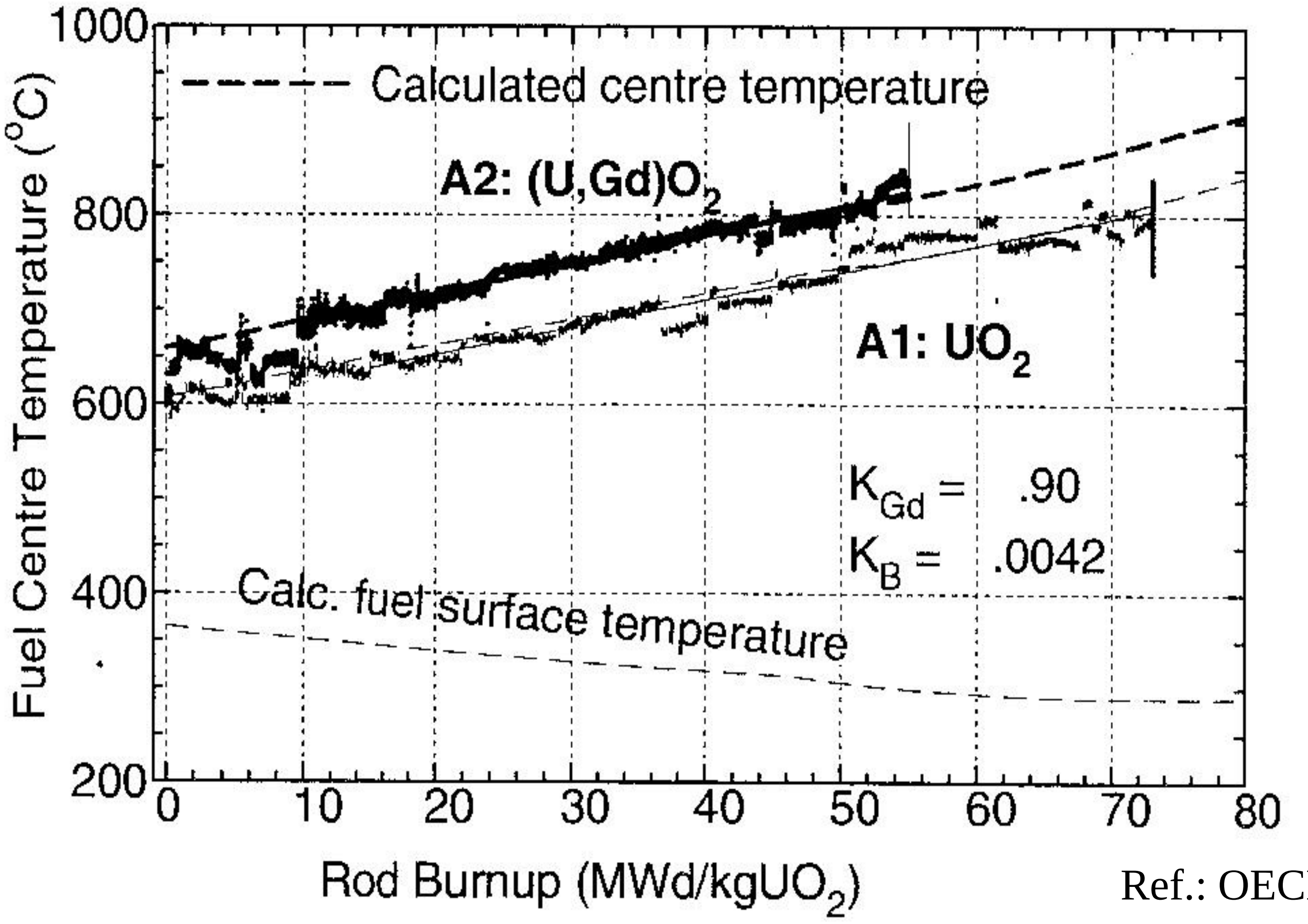
$$\left.\begin{matrix}\text{Composition}\\ \text{Irradiation}\end{matrix}\right\} \quad \mathrm{A} = \mathrm{A}(\text{composition, bu})$$

Effect of porosity on thermal conductivity of UO_2



Thermal conductivity degradation and effect of Gd

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



Ref.: OECD-HRP

General outline

REDUCTION OF RADIOLOGICAL CONSEQUENCES
OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Basic equations and limitations
  - Heat transfer
  - Mechanical analysis
  - Fission gas behaviour
- Coupling of modelling / experimental data

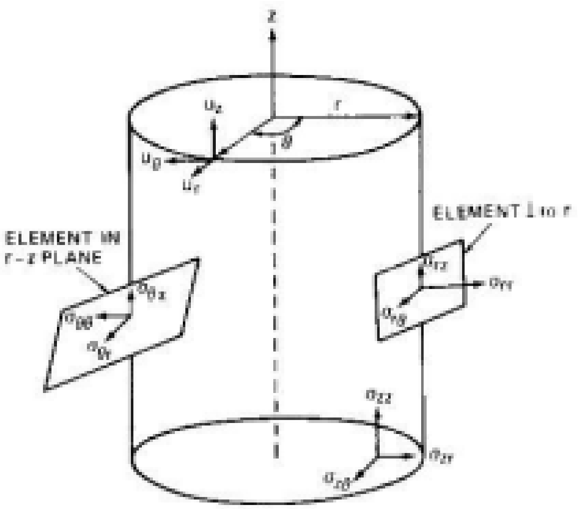
Mechanical analysis
Main assumptions

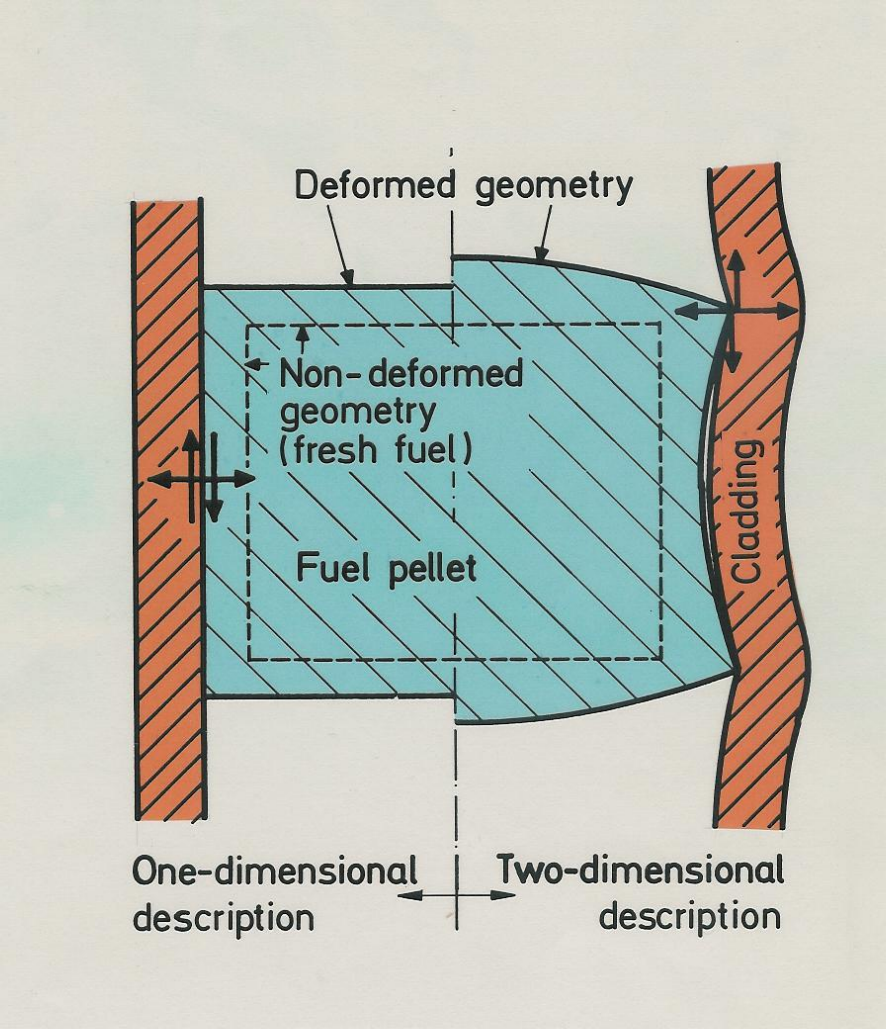
1. System is *axysimmetric*: no tangential variation

2. *Plane strain*:

   → Rod remains cylindrical

   → 1D problem





Constitutive relations

In general fuel and cladding are not only subject to elastic strains

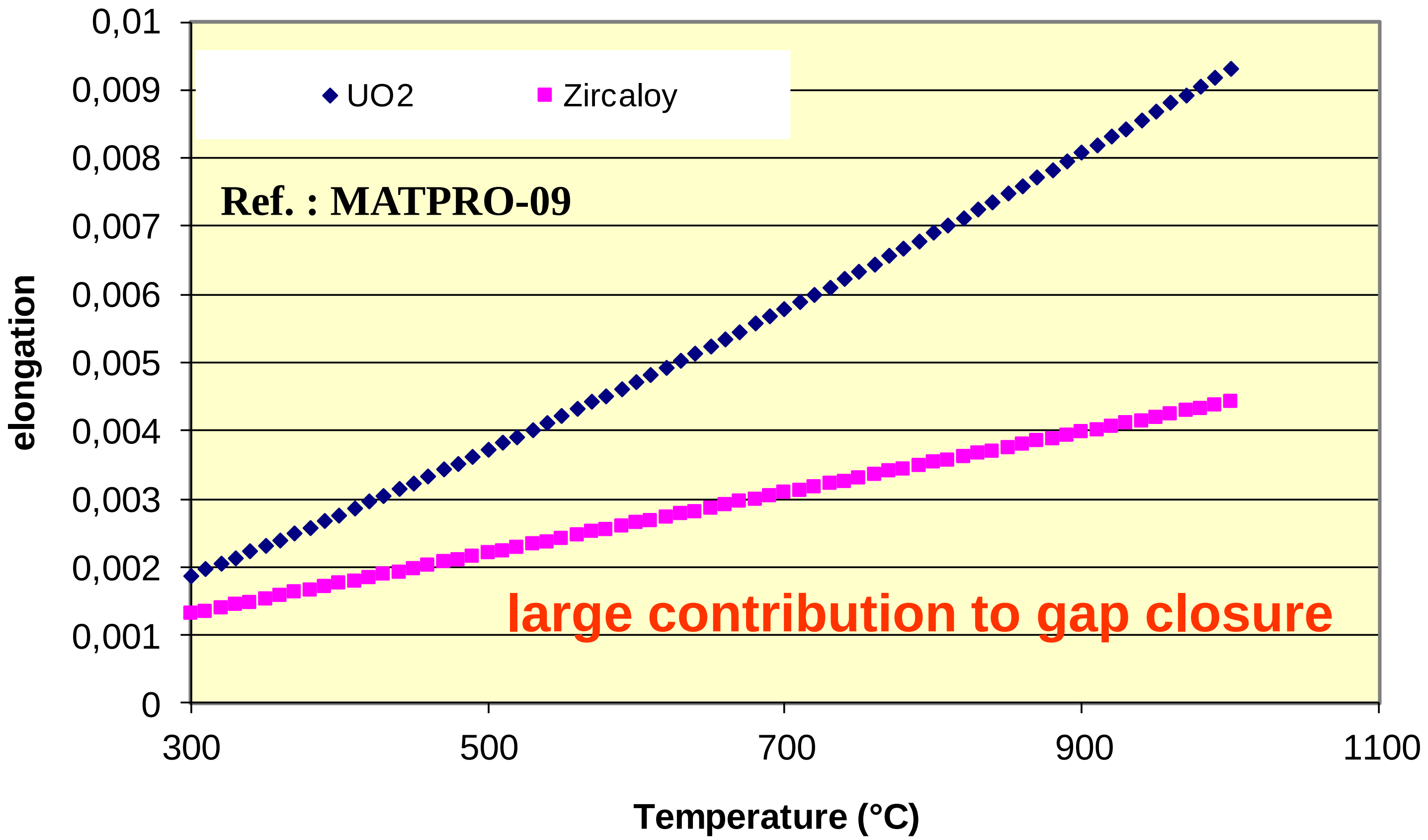
$$
\begin{cases}
\varepsilon_r^{tot} = \varepsilon_r^{e} + \varepsilon^{t} + \varepsilon^{s} + \varepsilon_r^{c} \\
\varepsilon_t^{tot} = \varepsilon_t^{e} + \varepsilon^{t} + \varepsilon^{s} + \varepsilon_t^{c} \\
\varepsilon_a^{tot} = \varepsilon_a^{e} + \varepsilon^{t} + \varepsilon^{s} + \varepsilon_a^{c}
\end{cases}
$$

Reversible
- Elastic strain
- Thermal expansion (isotropic)

Irreversible
- Swelling (isotropic)
- Deformation due to visco-plastic flow

Calculation of strains
Thermal expansion

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



Calculation of strains
Swelling

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

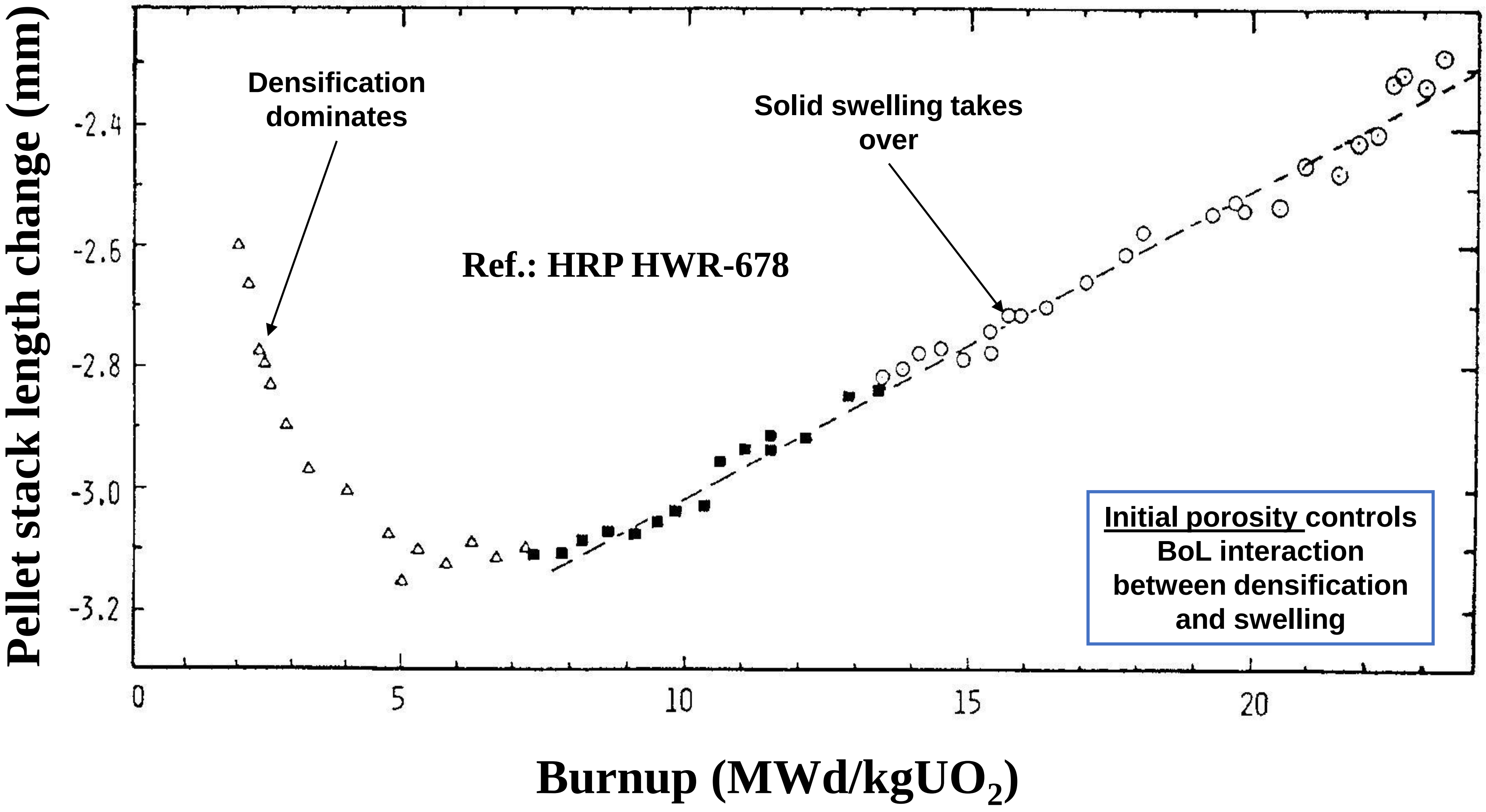
- We assume that swelling is isotropic
- Four contributions in fuel

$$\varepsilon^{s}_{fuel} = \frac{1}{3}\left[\left(\frac{\Delta V}{V}\right)_{solid\ FP} + \left(\frac{\Delta V}{V}\right)_{gaseous\ FP} - \left(\frac{\Delta V}{V}\right)_{densification} - \left(\frac{\Delta V}{V}\right)_{hot\ pressing}\right]$$

1. Inexorable swelling due to solid FP
2. Gaseous FP swelling
3. Reduction in volume by densification / sintering
4. Reduction in volume by hot pressing

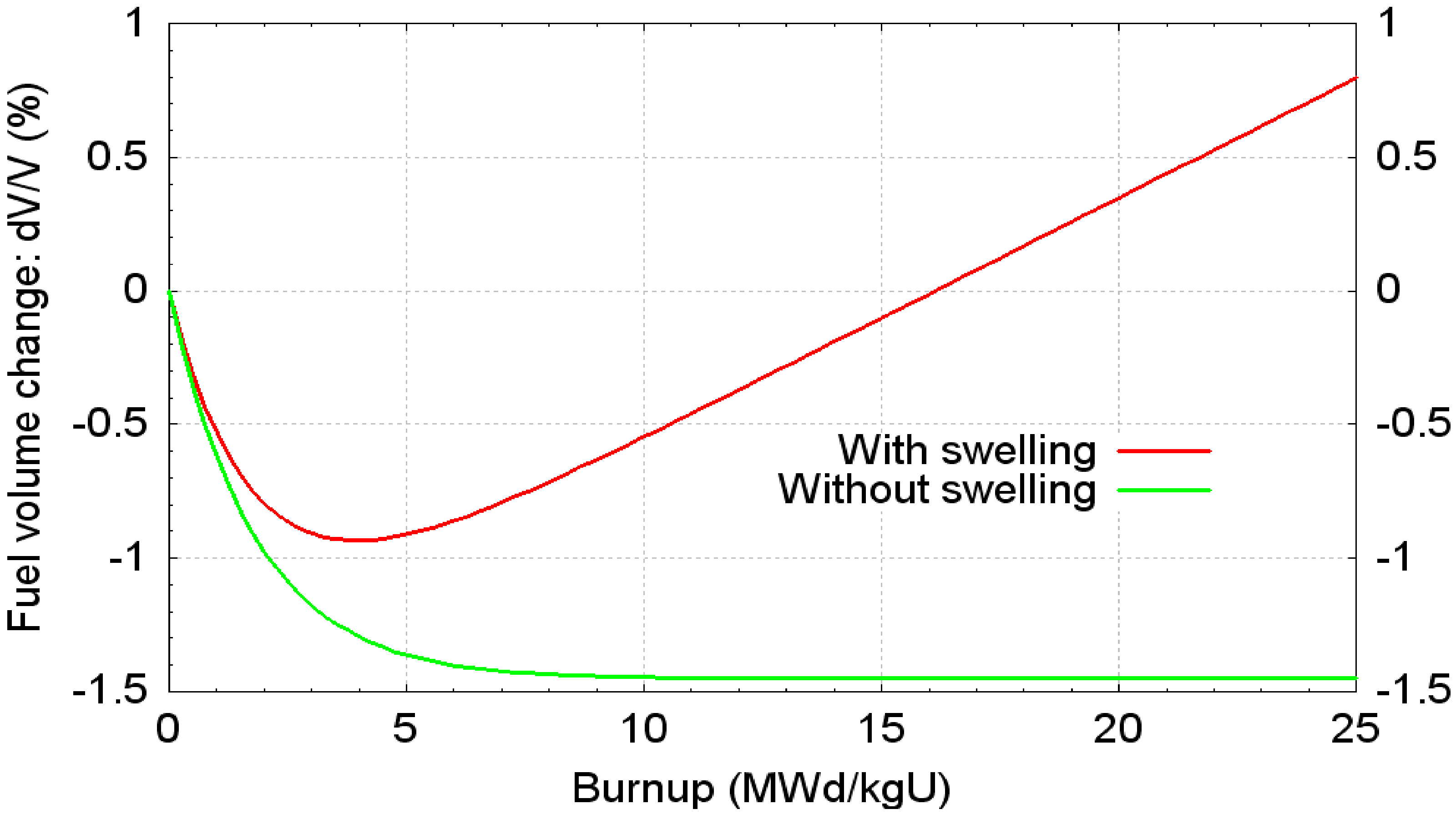
Hot standby stack length changes
densification +solid FP swelling

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



Modelling densification + swelling

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



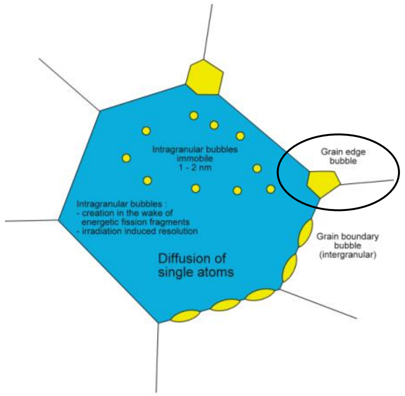
Modelling UO_2 swelling

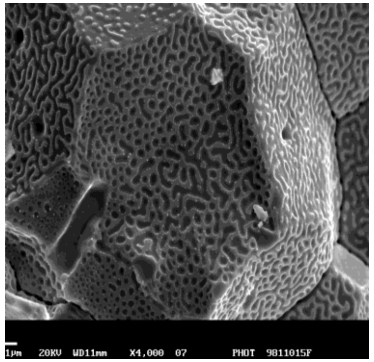
REDUCTION OF RADIOLOGICAL CONSEQUENCES
OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

Simple linear swelling due to FP accumulation

$$\Delta\left(\frac{\Delta V}{V}\right) = S\Delta Bu$$

Mechanistic gaseous swelling calculation (SCIANTIX of MFPR-F)





$$\left(\frac{\Delta V}{V}\right) = \left(\frac{\Delta V}{V}\right)_{FP} + \left(\frac{\Delta V}{V}\right)_{GB}$$

Calculation of strains
Visco-plastic strain: generalities

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Permanent deformation at constant volume

  → incompressibility condition:

$$\varepsilon_r^c + \varepsilon_t^c + \varepsilon_a^c = 0$$

- Two components

$$\varepsilon_i^c = \varepsilon_i^{plastic} + \varepsilon_i^{creep}$$

  - Plastic deformation: instantaneous (often only in clad)
  - Creep deformation: dependent on time

Plastic strain
Determine the onset

→Yield function: Relies on invariant of deviatoric stress tensor

- Von Mises criterion in 1D for isotropic materials

$$\sigma_{eff} > \sigma_{Yield}$$

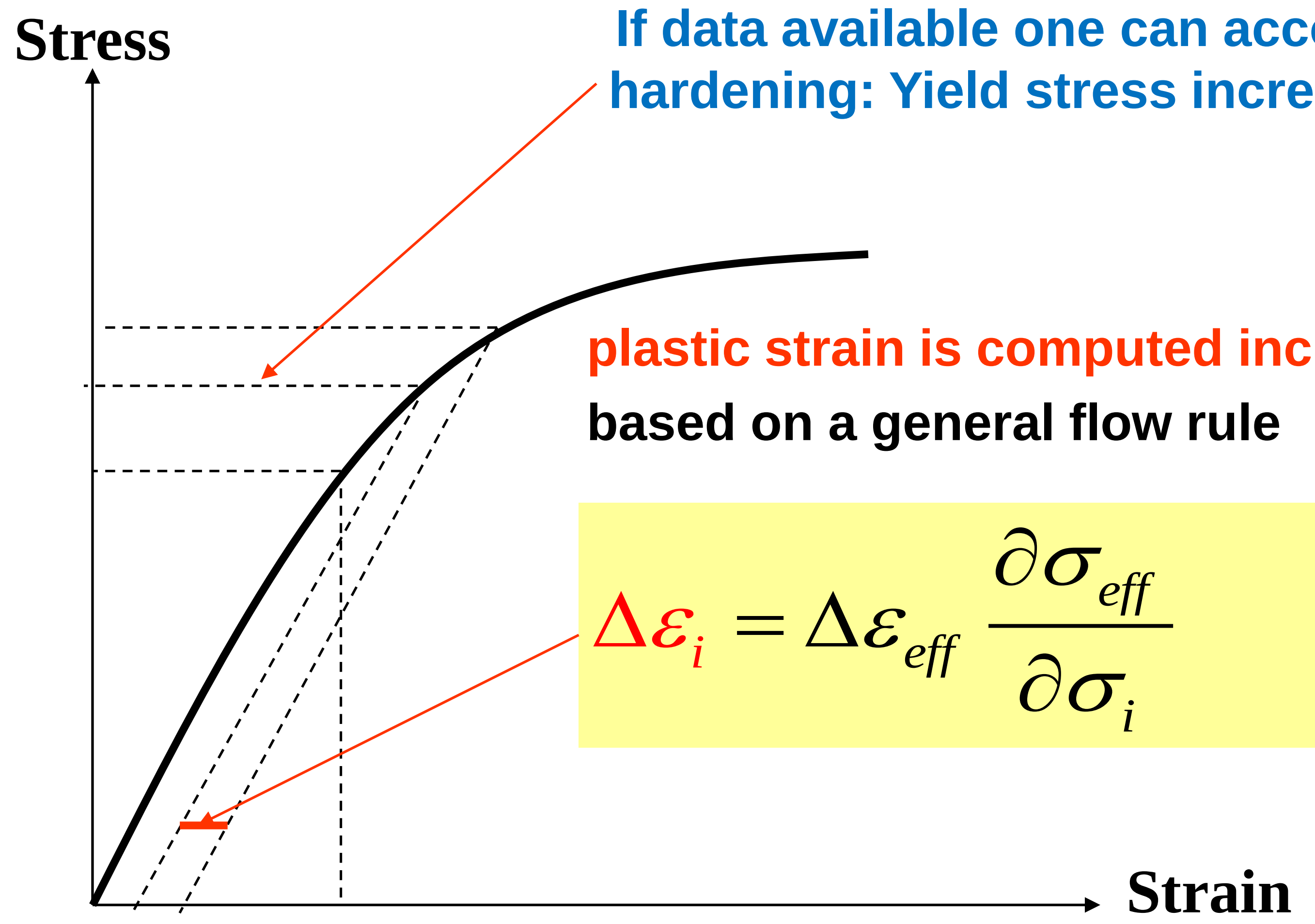
- depends on three principle deviatoric (shear) stresses

$$\sigma_{eff} = \frac{1}{\sqrt{2}}\left[(\sigma_r - \sigma_t)^2 + (\sigma_r - \sigma_a)^2 + (\sigma_t - \sigma_a)^2\right]^{1/2}$$

- Improvements:
  - Anisotropy coefficients (Hill's methodology)
  - Multi-dimensional yield surface

Plastic strain
Determine the onset

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



If data available one can account for strain hardening: Yield stress increases with time

plastic strain is computed incrementally
based on a general flow rule

$$\Delta\varepsilon_i = \Delta\varepsilon_{eff} \frac{\partial\sigma_{eff}}{\partial\sigma_i} \qquad i \in \{r, t, a\}$$

Calculation of creep strains

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

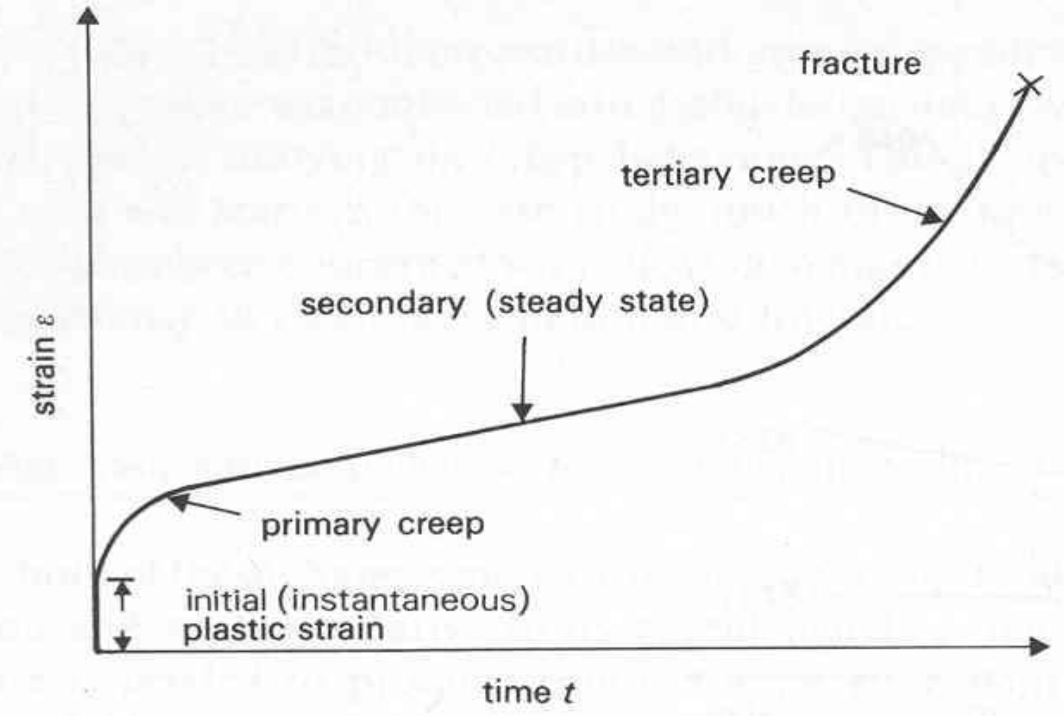
Components:

- **Thermal creep**
- **Irradiation induced creep**

Creep rate:

$$\dot{\varepsilon}_{eff} = f\left(T, \sigma_{eff}, \Phi\right)$$

Stages



Calculation of strains
Fuel cracking: description

- Occurs at startup due to differential thermal expansion:

  pellet centre expands more than pellet periphery

- Thermal stress in perfect cylinder (parabolic T):

$$\sigma_{t,\max} = \sigma_{a.\max} = -\frac{\alpha E\left(T_{f,c} - T_{f,s}\right)}{2(1-\upsilon)} - \frac{\alpha E q'}{8\pi(1-\upsilon)\bar{\lambda}}$$

E = 200 GPa, ν = 0.31 , $\bar{\lambda}$ = 3 W/mK, σ_{max} = 130 MPa

→ $T_{f,c}$-$T_{f,s}$ = 100°C or q' = 5 kW/m

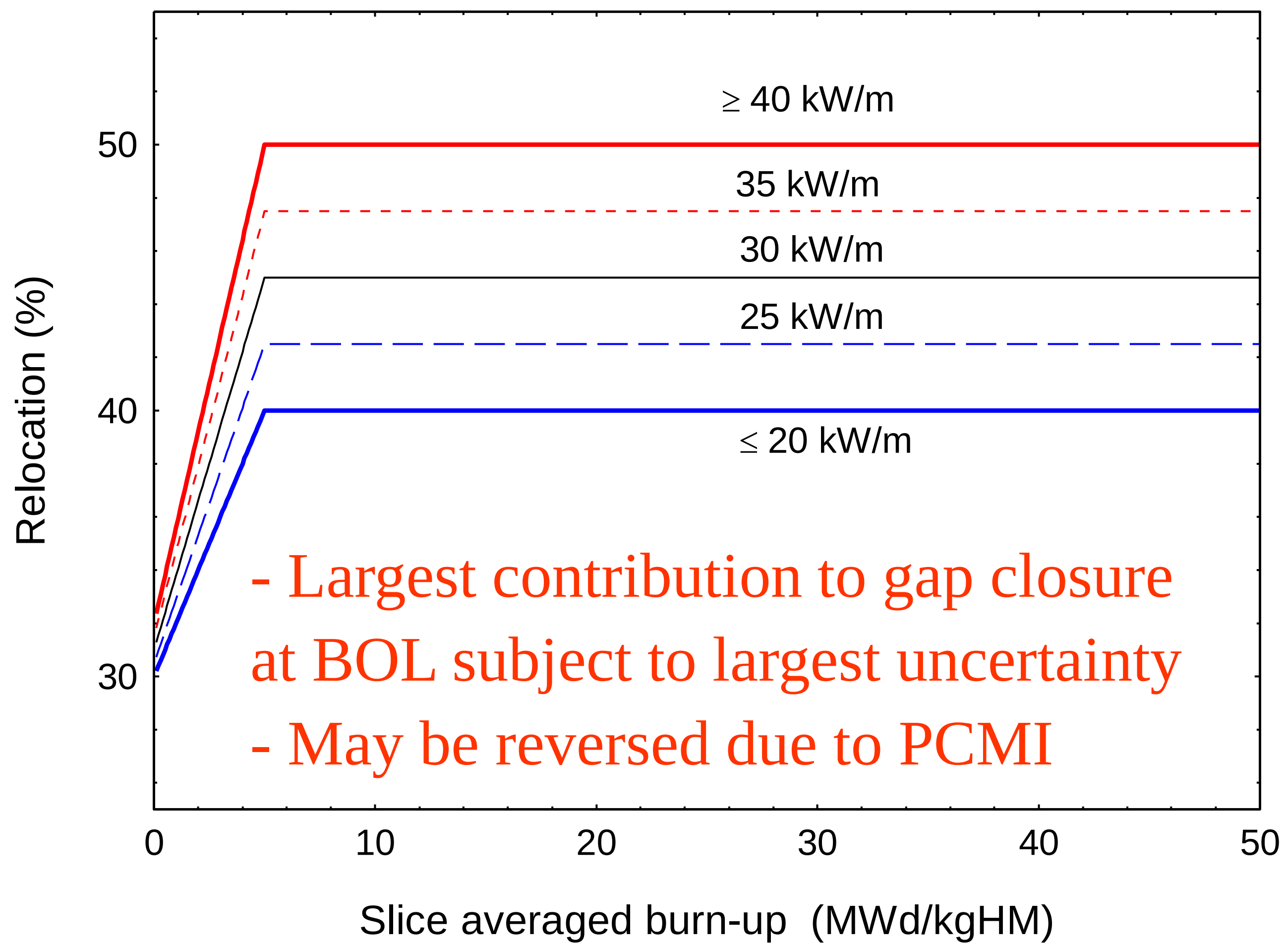
Calculation of strains
Cracking of fuel - Consequences

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Thermal analysis
  - Reduce fuel-cladding gap: relocation
- Mechanical analysis
  - Stress reduction, e.g. at interfaces: $\sigma = - P_{gas}$

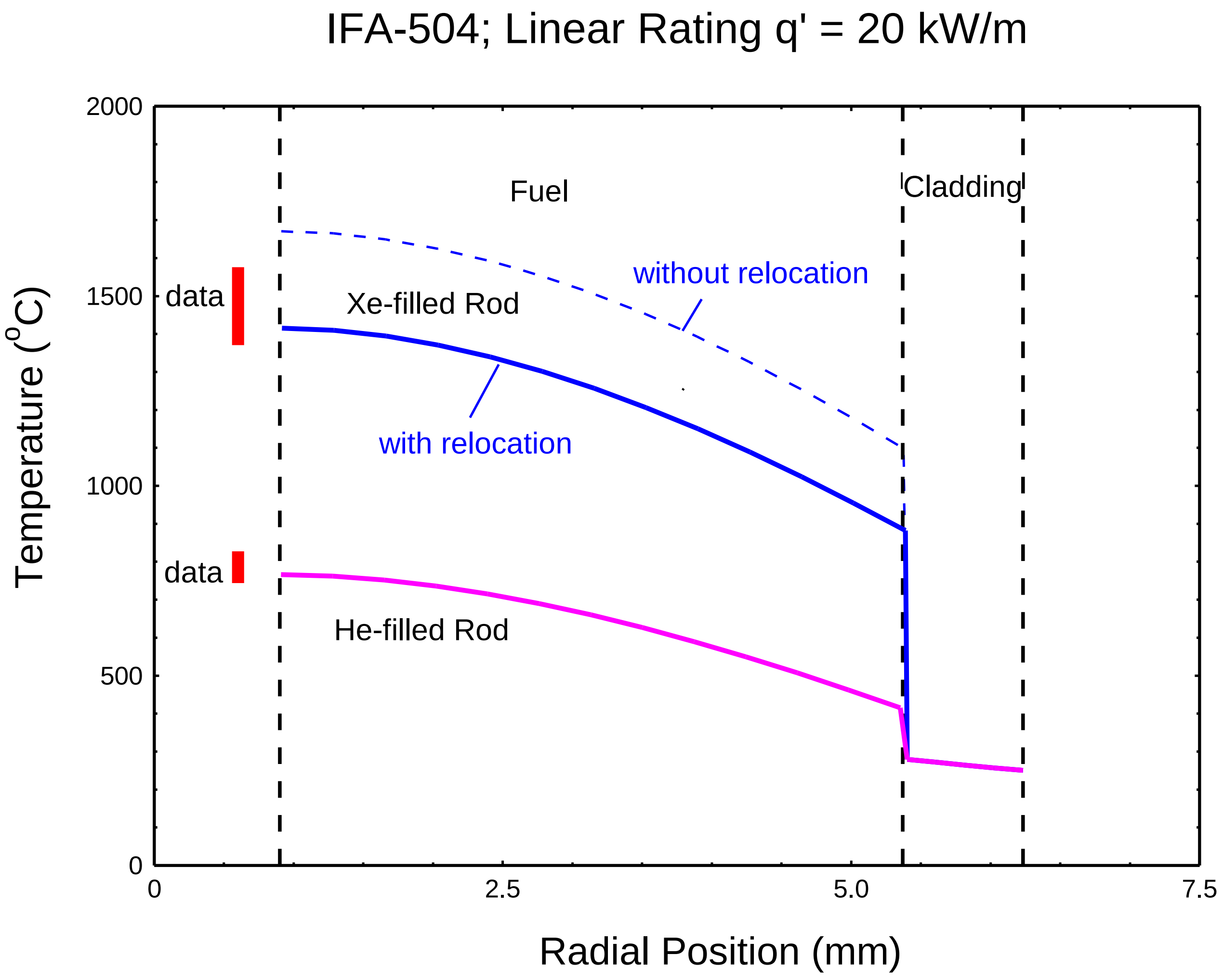
Calculation of strains
Cracking of fuel - Consequences

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



Cracking of fuel
Consequences of relocation on T

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



Calculation of strains
Cracking of fuel - Problems

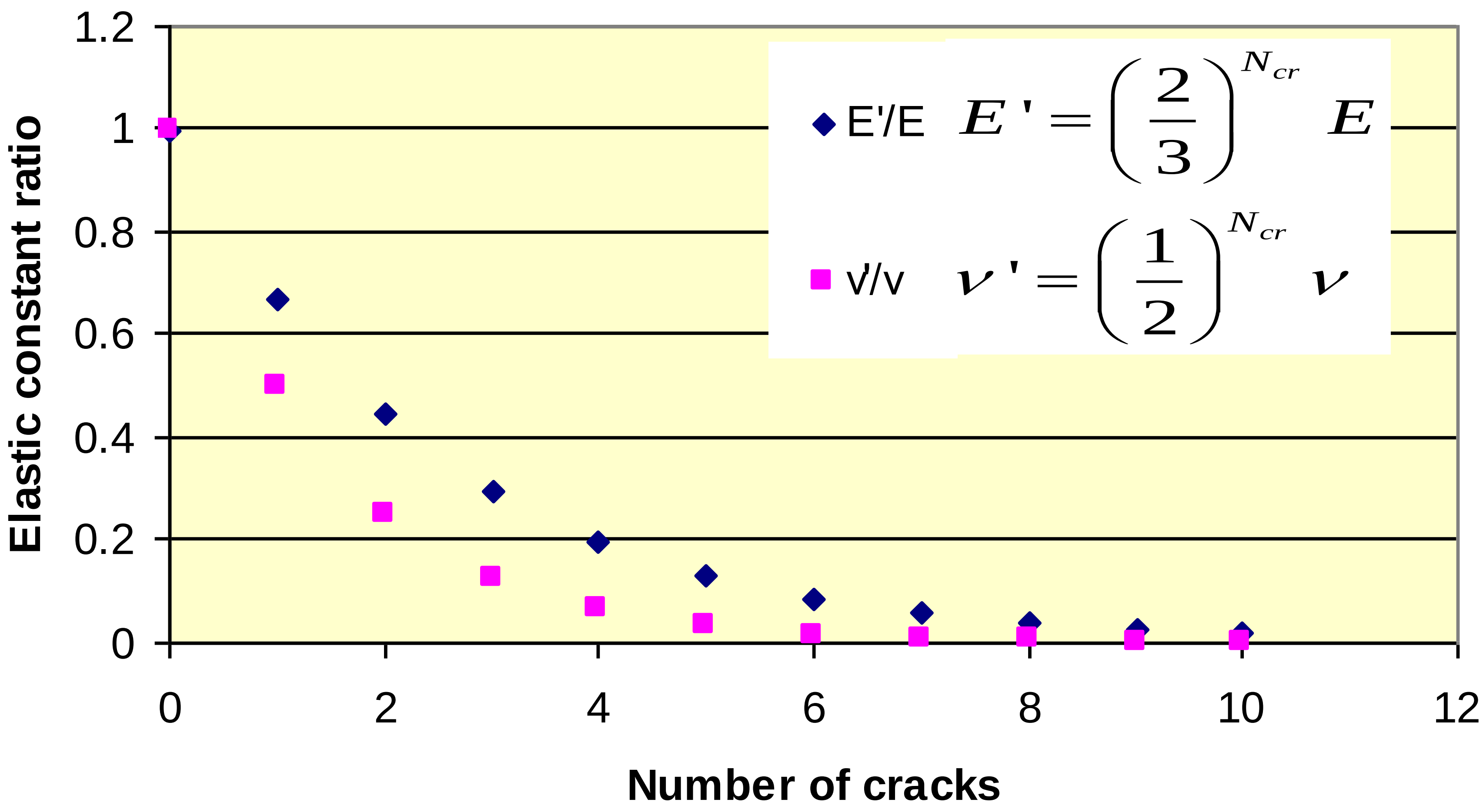
- Large uncertainty on rupture stress
  - Only obtained from uni-axial tensile tests
  - Effects of porosity, grain size and temperature
- Change of pellet geometry → loss of symmetry
  - Assumption invalid
  - Compression → tension in center

Calculation of strains
Cracking of fuel - Solutions

- T-distribution
  - cracks do not modify flow direction → reduce gap
- Stress distribution
  - Exact solutions: NO, to do so requires
    - Know location and size of every crack …
    - Solution of 3D stress-strain problem in each block
  - Approximate solutions
    - Modify material constants
    - Supplementary strain

Effect of cracking: modified elastic constants (LIFE)

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



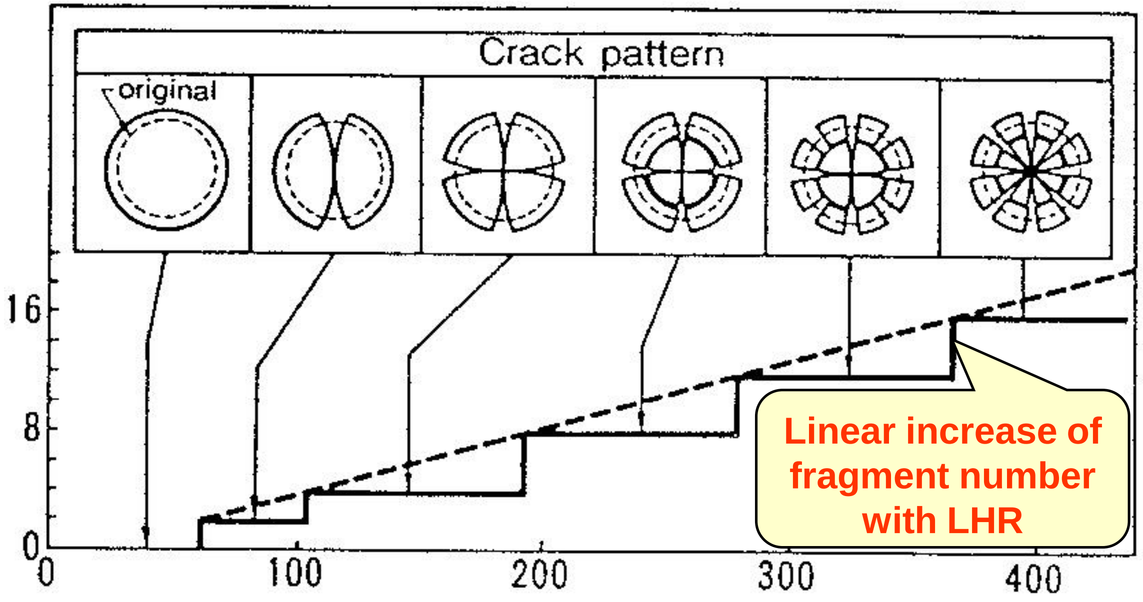
$$E' = \left(\frac{2}{3}\right)^{N_{cr}} E$$

$$\nu' = \left(\frac{1}{2}\right)^{N_{cr}} \nu$$

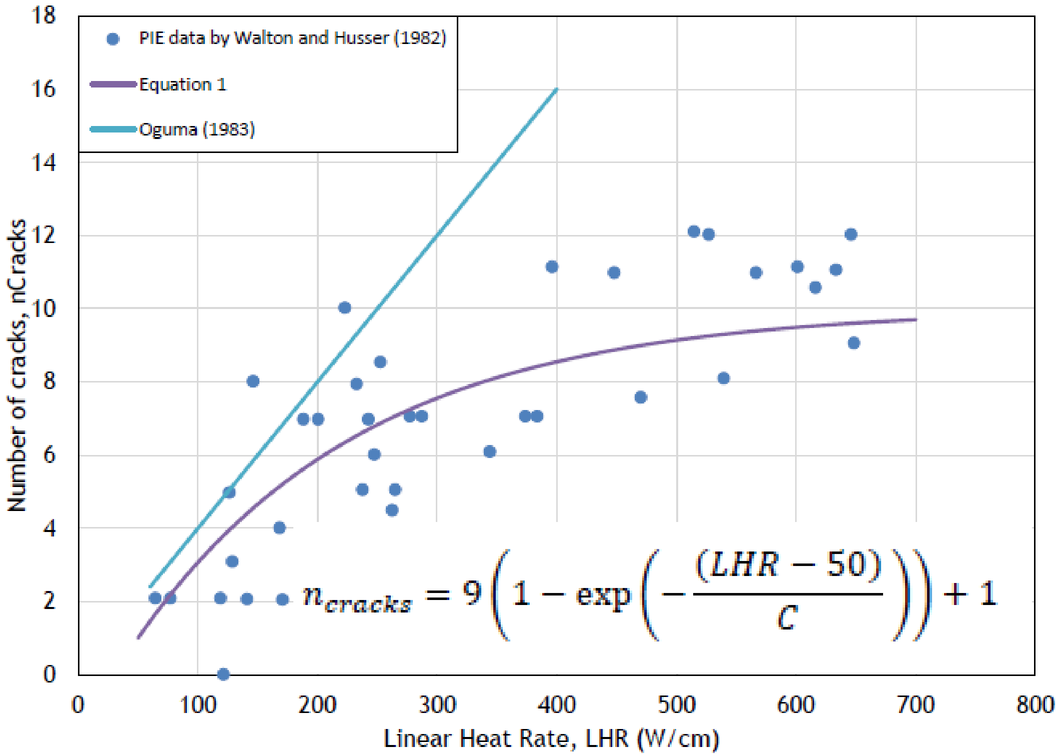
Pellet cracking: models for Nr of cracks

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

Oguma, NED, 1983



T. Barani, E. Bruschi, POLIMI, Italy, 2015



$$n_{cracks} = 9\left(1 - \exp\left(-\frac{(LHR - 50)}{C}\right)\right) + 1$$

Available e.g. in BISON, TRANSURANUS

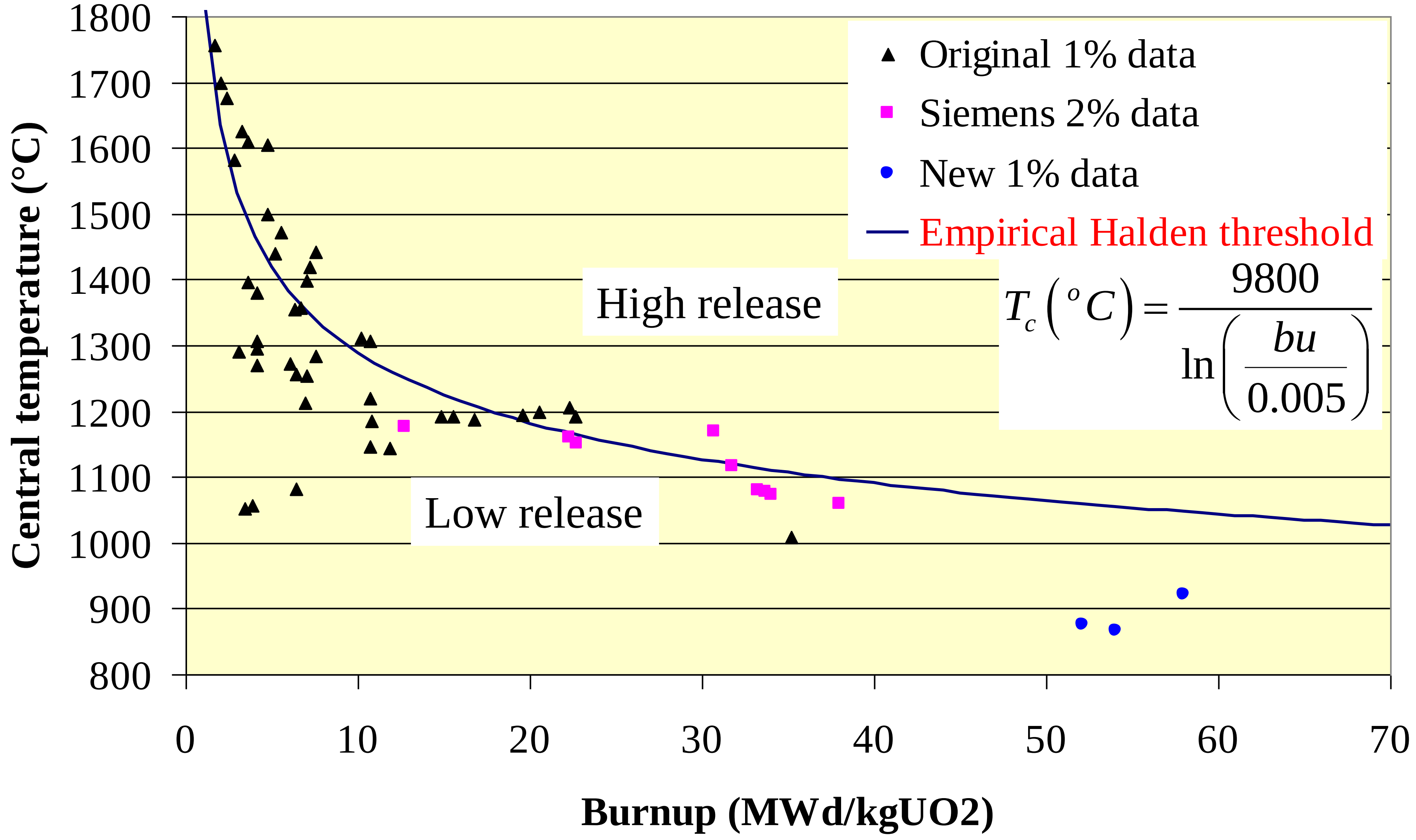
General outline

REDUCTION OF RADIOLOGICAL CONSEQUENCES
OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Basic equations and limitations
  - Heat transfer
  - Mechanical analysis
  - Fission gas behaviour
- Coupling of modelling / experimental data

Bubble interconnection leads to incubation

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS



Modelling of the FG behaviour

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

A two-step process

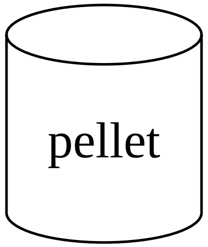
1. Intragranular behaviour: in the grains

2. Intergranular behaviour: along grain boundaries

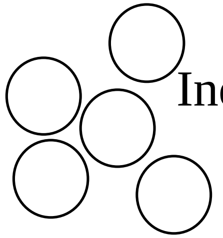
Intragranular FGR module
Booth model

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- polycrystalline sinter = collection of uniform spheres (Booth sphere)



$$R_B = 3\left(\frac{V}{S}\right)_t$$



Individual grains

No open porosity $\quad 3\left(\frac{V}{S}\right)_{geom} \geq R_B \geq R_{grain} \quad$ 100% open porosity

- atomic diffusion in hypothetical sphere
- grain boundary = perfect sink (gas immediately released)

Intragranular FG behaviour
Limitations of the Booth model

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

1. constant T and fission rate density
2. disregard resolution/trapping at intragr. bubbles
3. disregard grain boundary sweeping
4. cannot reproduce incubation (Vitanza curve)
5. disregard resolution at gb bubbles

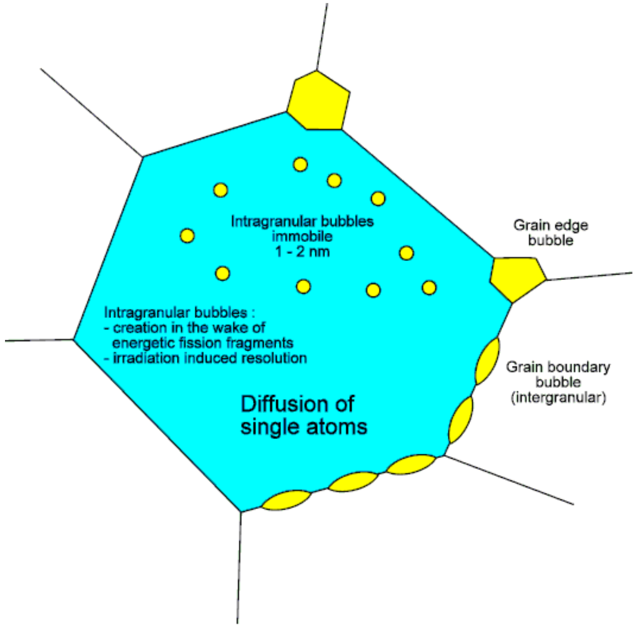
Alleviate limitation 2 of Booth model
Effective diffusion coefficient (Speight)

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Bubbles stabilize rapidly in size and number density
- Proposed model

$$\frac{\partial C_m}{\partial t} = D\Delta C_m + S - gC_m + bC_b$$

$$\frac{\partial C_b}{\partial t} = gC_m - bC_b$$



- Saturated traps

$$\frac{\partial (C_m + C_b)}{\partial t} = D\Delta C_m + S = \frac{b}{b+g} D\Delta (C_m + C_b) + S$$

$$= D_{eff}\Delta (C_m + C_b) + S$$

Alleviate limitation 2 of Booth model
NEW Effective diffusion coefficient

- Consider bubble diffusion

$$\frac{\partial C_m}{\partial t} = D_m \Delta C_m + S - gC_m + bC_b$$

$$\frac{\partial C_b}{\partial t} = gC_m - bC_b + D_b \Delta C_b$$

$$\frac{\partial (C_m + C_b)}{\partial t} = \left[\frac{b}{b+g} D_m + \frac{g}{b+g} D_b \right] \Delta (C_m + C_b) + S$$

$$= D_{eff} \Delta (C_m + C_b) + S$$

Gas atom diffusion coefficient

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

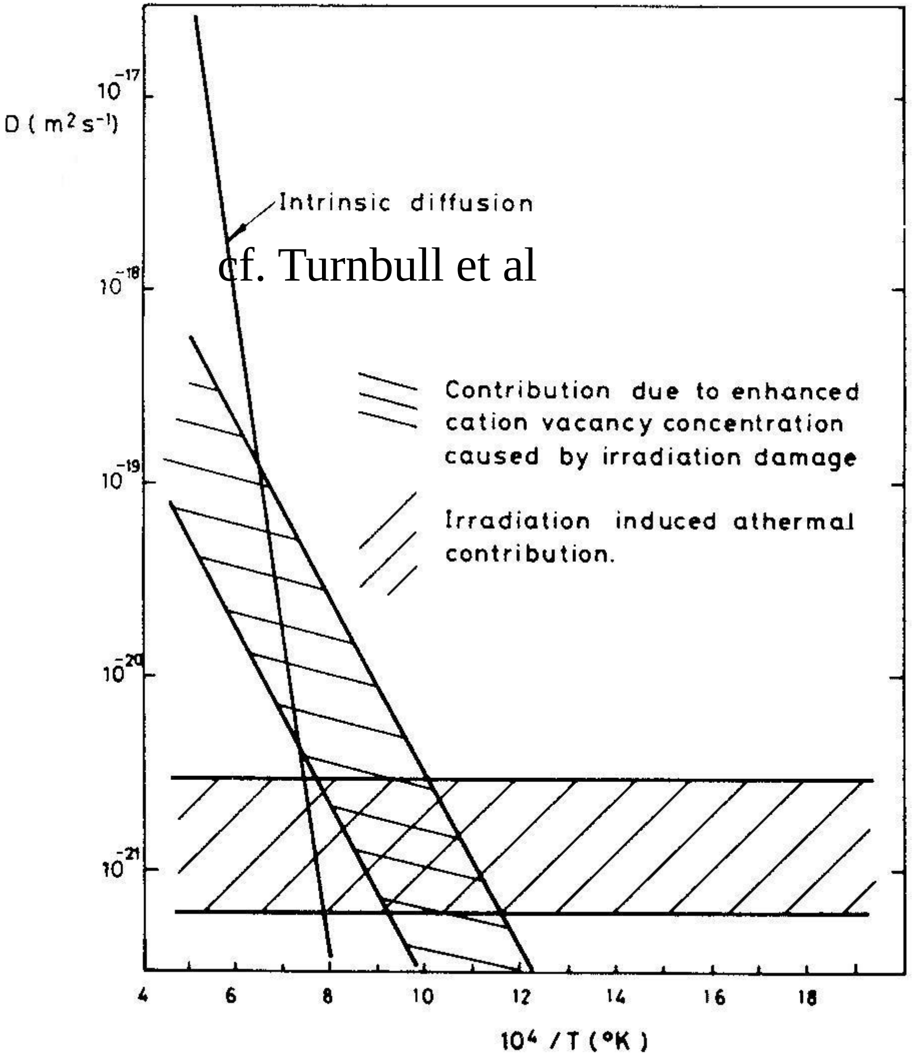
Three temperature regimes

$$D_1 = 7.6 \cdot 10^{-6} \exp\left(-\frac{35000}{T}\right)$$

$$D_2 = 5.6 \cdot 10^{-25} \cdot \sqrt{\dot{F}} \exp\left(-\frac{13800}{T}\right)$$

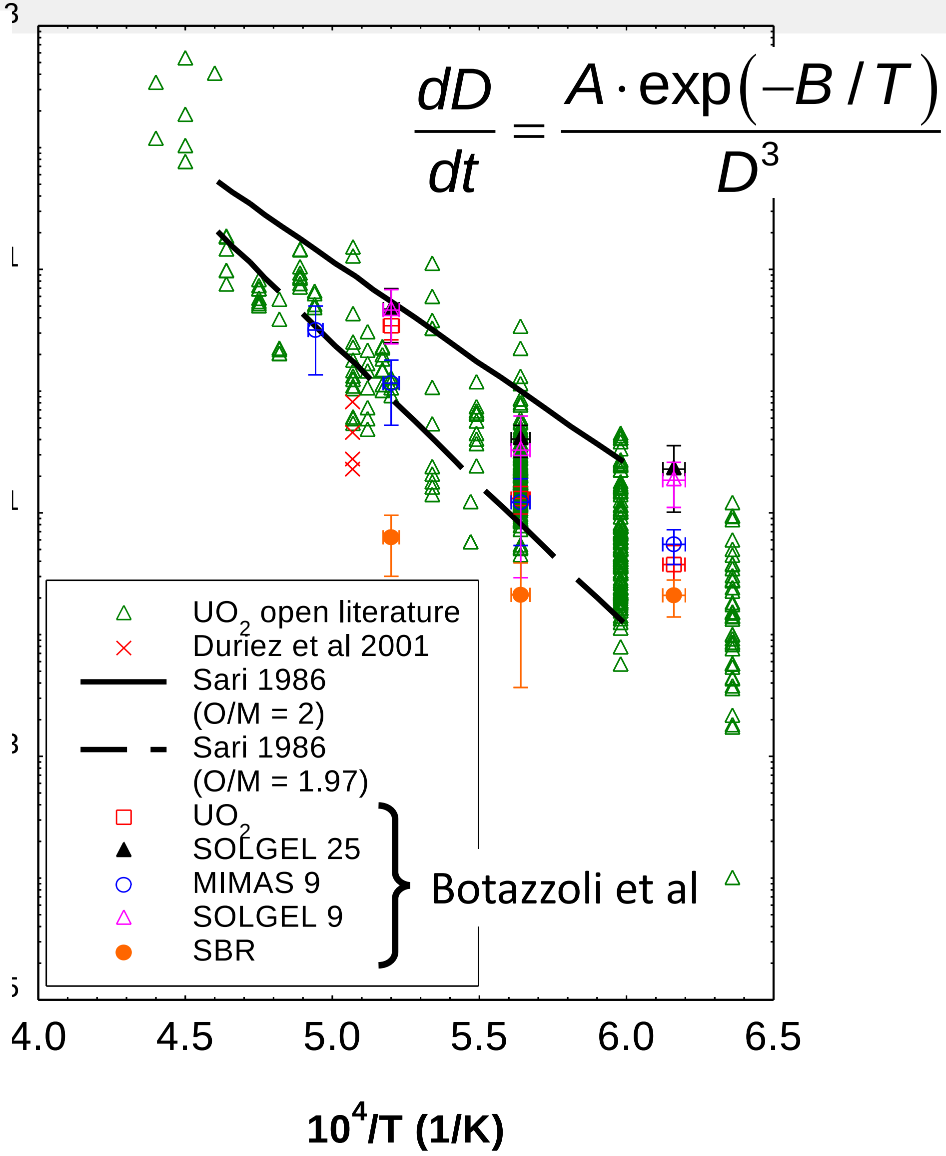
$$D_3 = 8 \cdot 10^{-40} \cdot \dot{F}$$

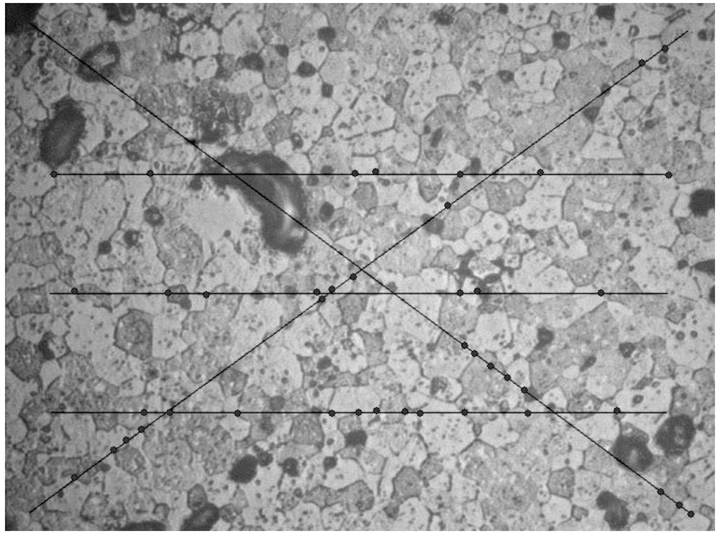
Large uncertainty: factor 5↑or↓



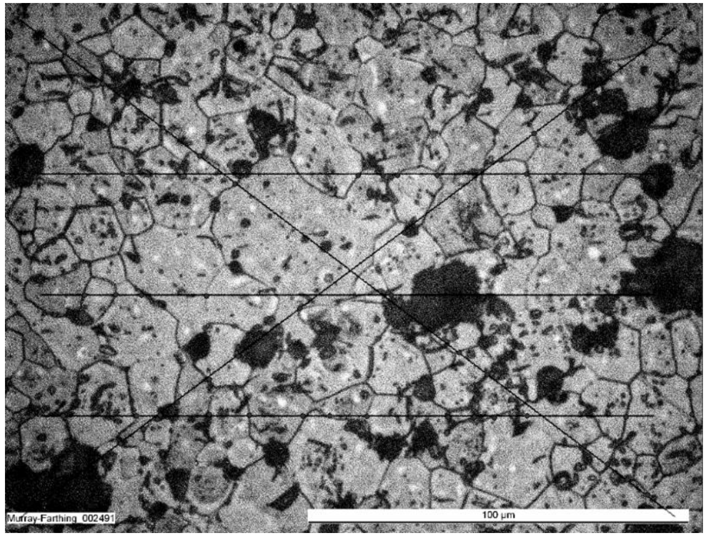
Grain growth in MOX and UO_2

$$\frac{dD}{dt} = \frac{A \cdot \exp(-B/T)}{D^3}$$





Before annealing



After annealing

Modelling the FG behaviour

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

A two-step process

1. Intragranular behaviour: in the grains

2. Intergranular behaviour: along grain boundaries

   → alleviate limitations 4 and 5 of Booth model

Coupling with intragranular module
Boundary condition in intragranular module

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

Zero BC	Non-zero BC
↓	↓
segregation factor is ∞, or the gb is a thermodynamic perfect sink (simplest)	segregation factor reflects the interaction energy of solute atoms with the gb
Majority of models	Turnbull et al, Olander et al, Forsberg and Massih, Van Uffelen

Fission gas behaviour
Swelling

REDUCTION OF RADIOLOGICAL CONSEQUENCES
OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Mostly empirical model

$$\left(\frac{\Delta V}{V}\right)_{gaseousFP} = A\left(1-\alpha_{FG}FGR-\alpha_{Cs}CSR\right)bu$$

- However, swelling should be linked to FGR via gas balance as typically done in mechanistic models (e.g. SCIANTIX, MFPR-F)

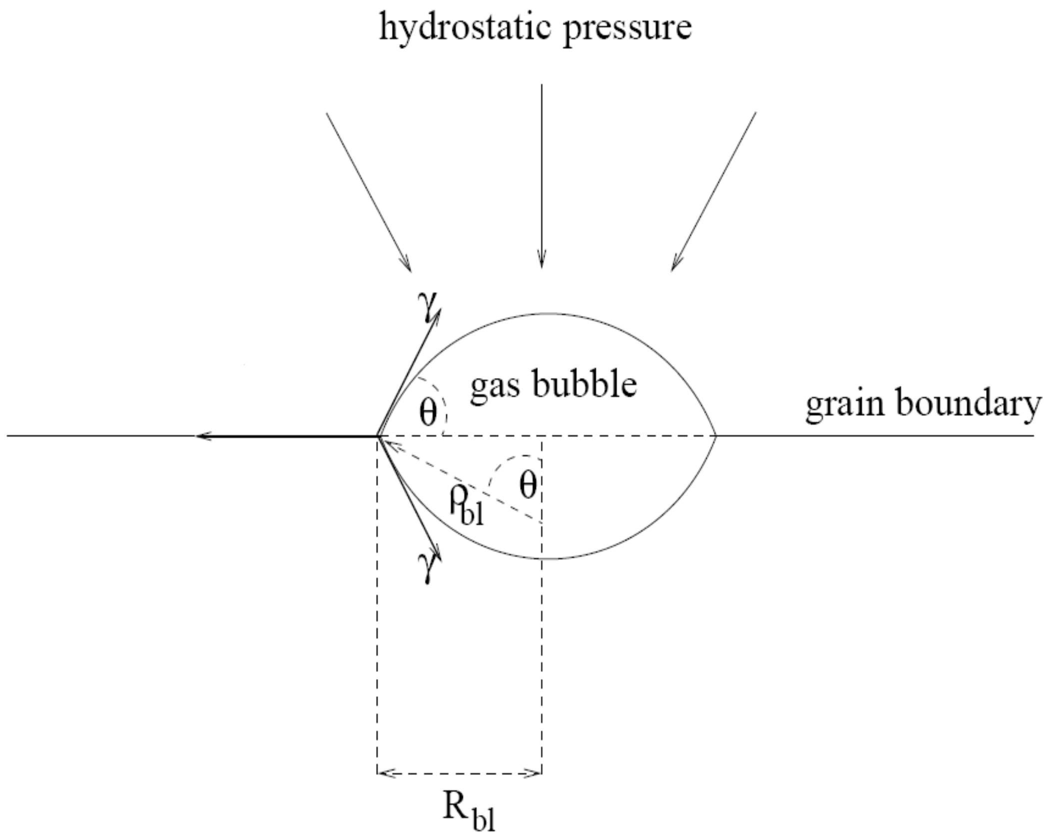
Fission gas behaviour

New swelling and release model (1)

REDUCTION OF RADIOLOGICAL CONSEQUENCES
OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

Basic assumptions for grain boundary model

- All gas retained inter-granular <u>bubbles</u>.
- bubbles have <u>uniform</u> size and lenticular shape



Fission gas behaviour

New swelling and release model (2)

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- Bubble growth/shrink by absorption/emission of vacancies

$$\frac{dn_{vac}}{dt} = \frac{2\pi D_g \delta_g}{kTS}\left(p - \frac{2\gamma}{R_{bubble}} - \sigma_h\right)$$

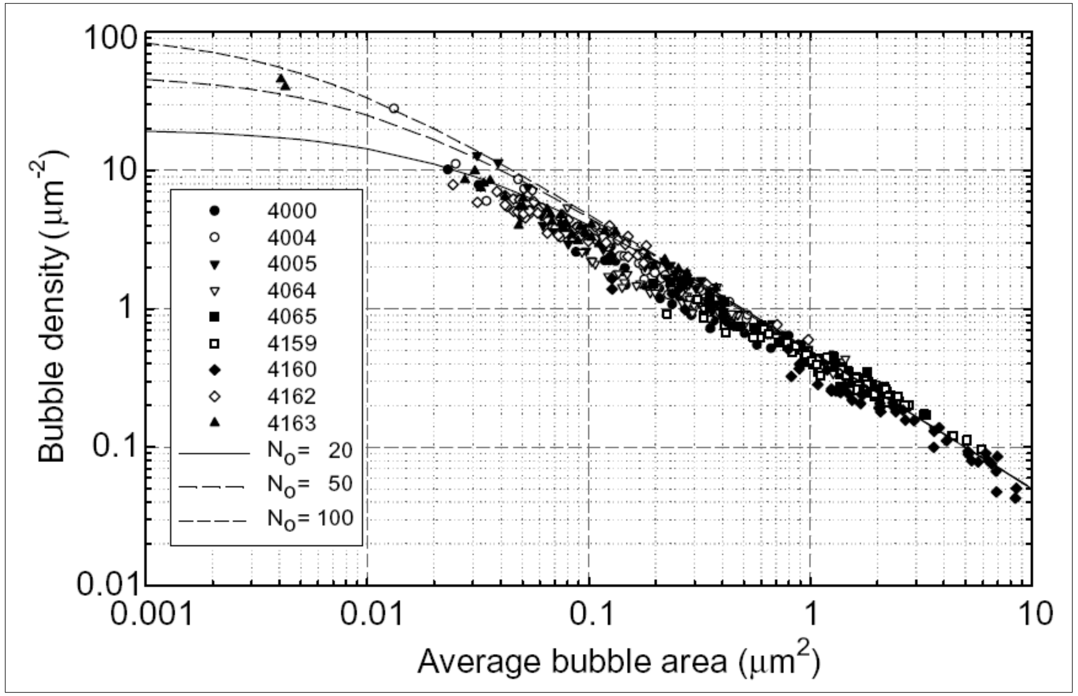
- Gas obeys Van der Waals equation of state

- Bubble coalescence

  determined by geometry

$$\frac{dN_{bubble}}{dA_{bubble}} = -2N_{bubble}^2$$

G. Pastore, PhD, POLIMI
R. White, IFPE database

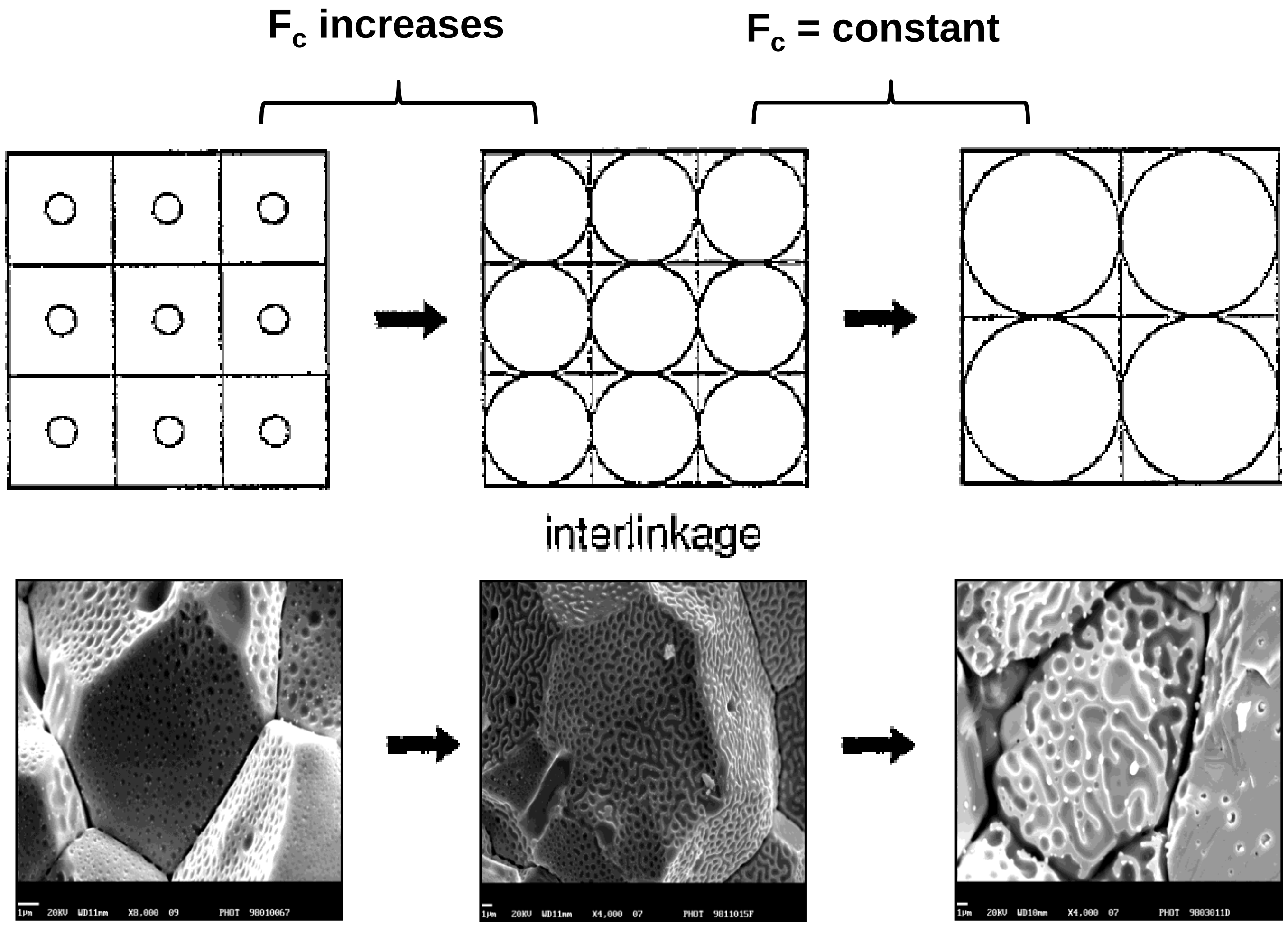


Fission gas behaviour

New swelling and release model (3)

REDUCTION OF RADIOLOGICAL CONSEQUENCES OF DESIGN BASIS & DESIGN EXTENSION ACCIDENTS

- <u>gas release</u> at saturation of grain boundary coverage



G. Pastore

Thank you!

Paul.Van-Uffelen@ec.Europa.eu

This project has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 847656.