Nuclear Fuel Performance

NE 533: Spring 2025

Last Time

- All reactors have basic requirements they must meet
- Typically, the “fuel system” is thought to consist of the fuel itself, the gap, the cladding, and the coolant
- Mining -> Processing -> Conversion -> Enrichment -> Powder -> Compaction/Sintering -> Rod/Assembly
- U_3O_8 must be converted to UF_6 for enrichment, which is then converted to UO_2 powder for pellet manufacture
- UO_2 microstructure from fabrication strongly impacts fuel performance

HEAT GENERATION

Calculating heat generation rate for a given fuel

- We know about 200 MeV of energy is available due to a fission (210 MeV minus neutrinos)
- We know the fission cross section of the target nuclide (tabulated)
- We know the neutron flux (given by reactor conditions)
- We can calculate the fission atom density
- The heat generation rate, Q is given by:
  - $Q = E_f \times N_f \times \sigma_f \times \phi$
  - Where E_f is the fission energy, N_f is the fission atom density, σ_f is the fission cross section, and ϕ is the neutron flux
  - Units: J/fission x atoms/cm^3 x (fission/neutron)*(cm^2/atom) x (neutron/cm^2-s) = J/cm^3-s = W/cm^3

Calculating heat generation rate for a given fuel

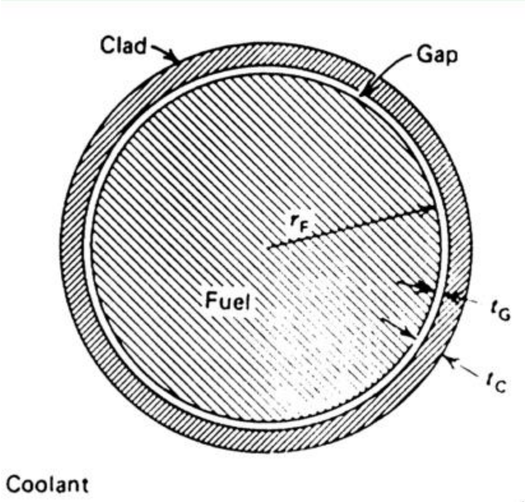
- Cross sections:
  - ENDF database: Nuclear Data Sheets 148 (2018) 1–142
  - Thermal neutron (E=0.025 eV) U235 fission cross section: ~586.8 barns
    - 1 barn = 10^{-24} cm^2
- Fission atom density
  - Atom density of U-235 = UO_2 density x 1/molar mass x Avogadro's number x atom fraction x enrichment

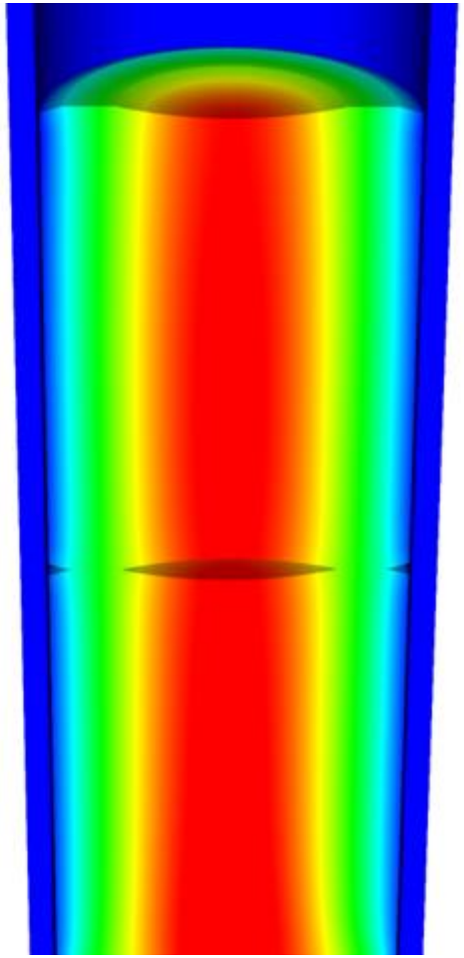
Example

HEAT TRANSPORT

Heat transport route

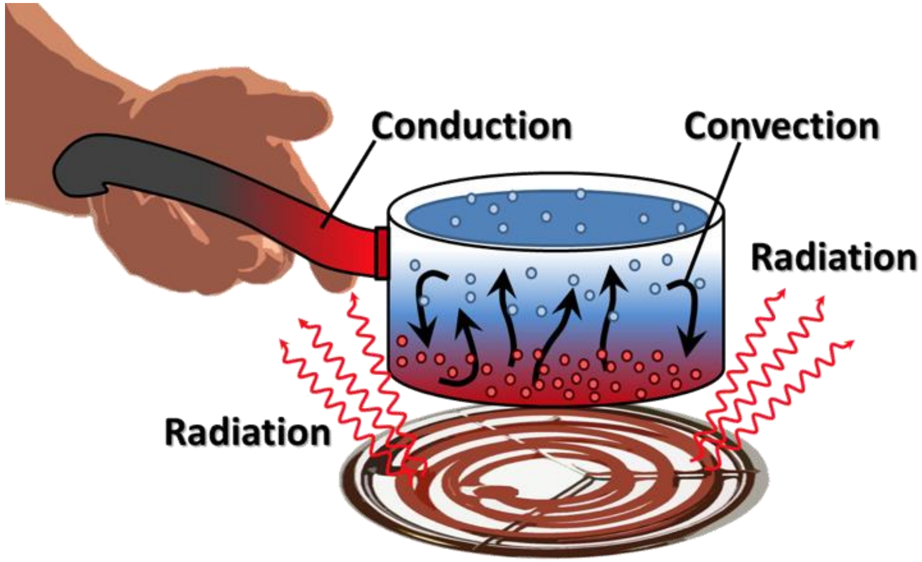
- Heat is produced in the fuel, transports through the cladding and gap, and into the coolant
- Important quantities include
  - Volumetric heat generation rate Q (W/cm^3)
  - Fuel Centerline temperature T_0
  - Surface temperature of the fuel T_S
  - Inner cladding temperature T_{IC}
  - Outer cladding temperature T_{OC}
  - Coolant temperature T_{cool}
  - Fuel pellet radius r_F
  - Gap thickness t_G
  - Cladding thickness t_c
  - Coolant heat transfer h_c





Heat can be transported in three ways

- Convection
  - Heat transfer through mass movement of liquid or gas
- Radiation
  - Heat transfer by means of photons in electromagnetic waves
- Conduction
  - Heat transfer by molecular, phonon, and electronic vibration/collisions



Heat transfer mode in fuel systems?

- How is heat transported through the fuel?

  Conduction

- How is the heat transported through the gap?

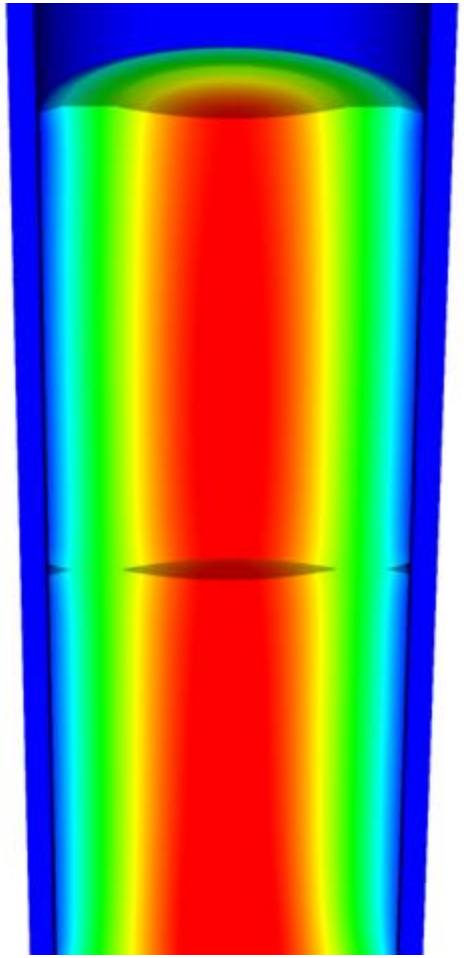
  Mostly conduction, some convection

- How is heat transported through the cladding?

  Conduction

- How is heat transported to the coolant?

  Convection



Heat conduction equation

- ρ is the density, c_p is the specific heat, T is the temperature, t is the time, and k is the thermal conductivity, Q is heat generation
- It is a partial differential equation in time and space of the temperature, T(**x**, t), where **x** is a vector defining the position in space
- What do we need to know to solve this equation?

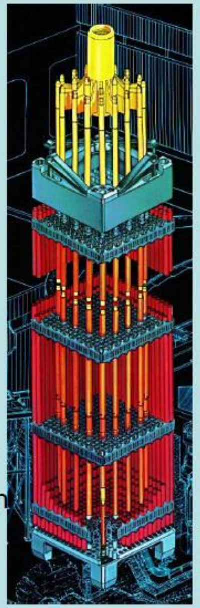
$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

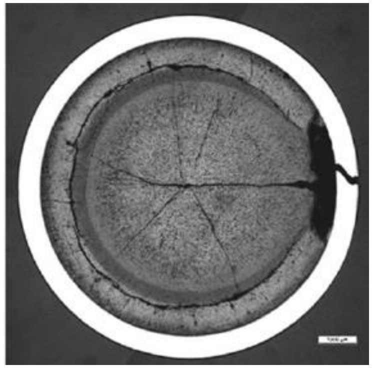
- The geometry of our problem
- The initial condition of T
- The boundary conditions of T
- Is each parameter is a function of T
- If they aren't a function of T, do they vary in space and time for some other reason?

What is our geometry for the problem?

- Reactor geometry depends on reactor type
- The idealized geometry of each fuel rod is axisymmetric, but in reality, it is 3D
- Fuel pellet defects cause 3D geometry
- The stacked pellets may not be stacked perfectly, causing their center axis to not be aligned, also causing 3D geometry

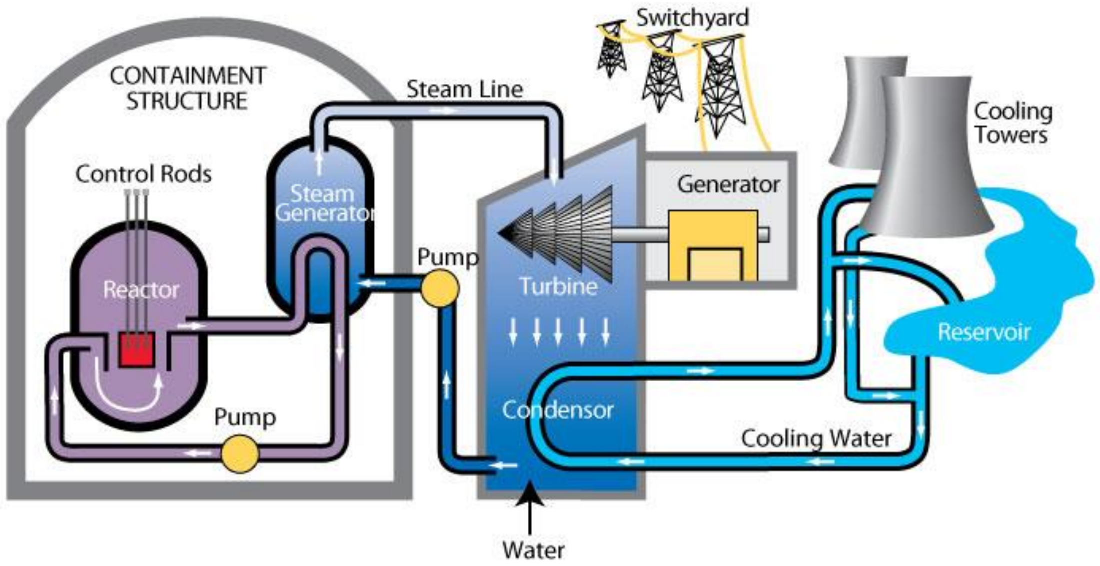
	BWR	PWR
Lattice	10x10	14x14 – 18x18
Lattice size	~5.3”	~9”
Height	120”-150”	144”-168”
Fuel	UO_2/MOx	UO_2/MOx
Fuel rods	~92	176-300
Part length rods	~14	0
Non-fueled rods	~2	20-25
Control	Ext. control rod	Int. control cluster
Cladding	Zr2 for PCI, nodular corrosion	Zr4/Zirlo/M5 for uniform corrosion & hydrogen
Channels	Yes	No
Fuel mass	~180 kgU	~600 kgU





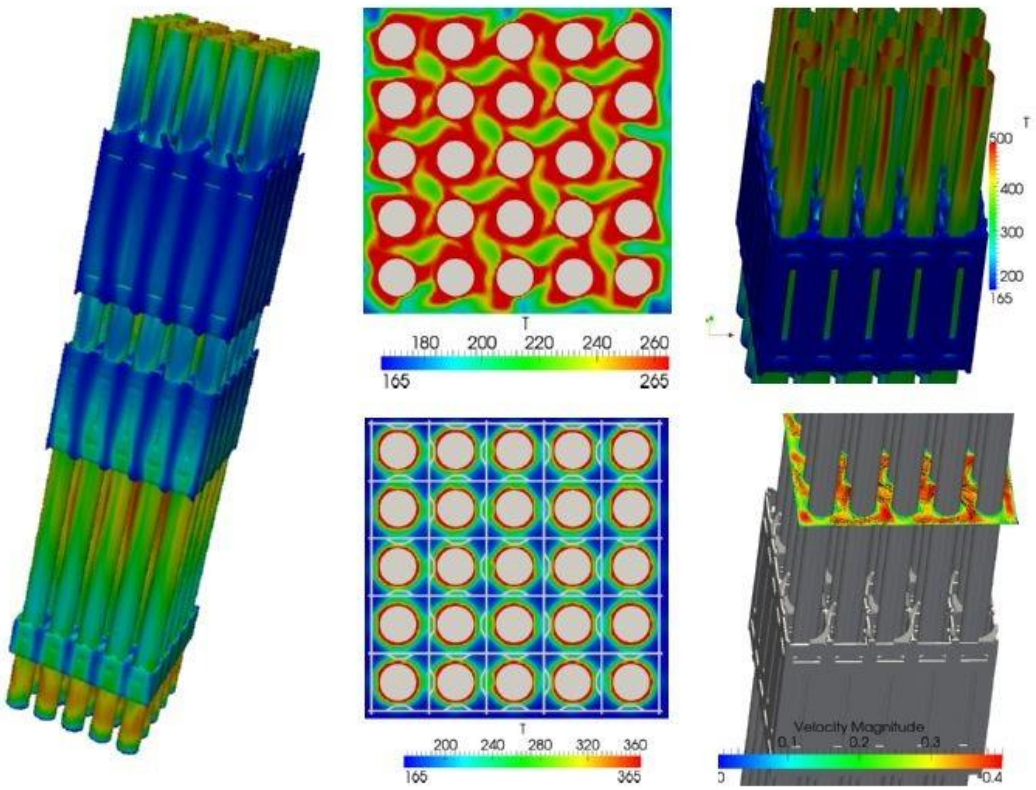
The initial condition of T

- The initial condition of T is set by the state of the reactor directly before startup (or before time of interest)
- The initial temperature is uniform throughout the fuel, equal to the initial coolant temperature
- $T(\mathbf{x}, 0) = T_{cool}(0)$



Boundary conditions?

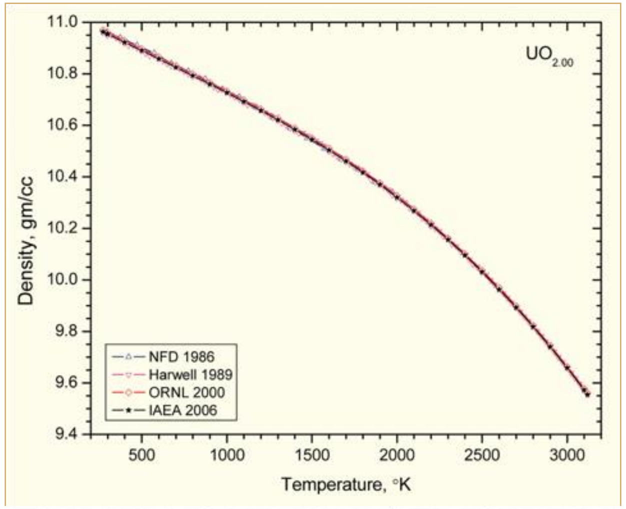
- The boundary conditions on T is set by the coolant flow
- The temperature of the coolant T_{cool} is complicated
  - It varies along the length of the fuel rod (axially)
  - It various around the circumference of the fuel rod

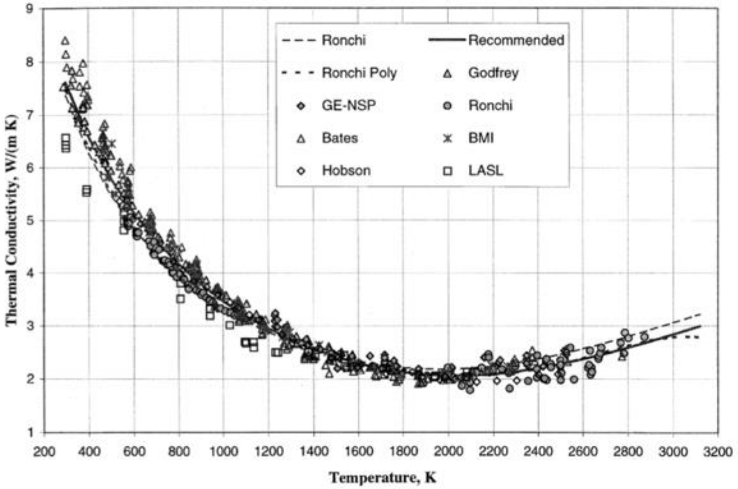


Fuel properties

- All properties vary as a function of composition, thus as a function of burnup/time
- Density varies as a function of T (thermal expansion)
- Thermal conductivity also varies with temperature

$$k_0 = \frac{100}{7.5408_{17.629T} + 3.6142T^2} + \frac{6400}{T^{5/2}} exp\left(\frac{-16.35}{T}\right)$$

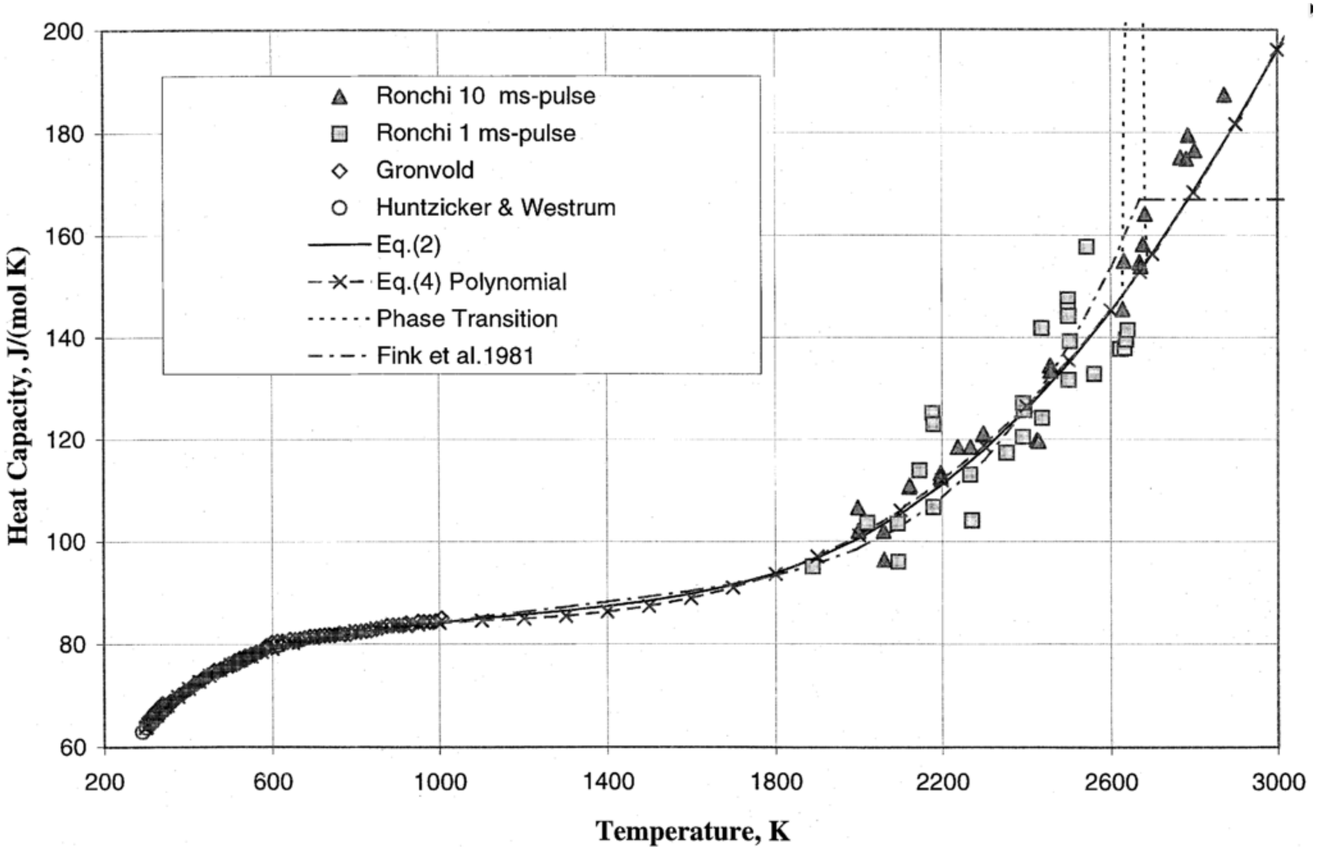




The heat capacity is a function of temperature

$$C_P = \frac{C_1\theta^2 e^{\theta/T}}{T^2(e^{\theta/T}-1)^2} + 2C_2T + \frac{C_3E_a e^{-E_a/T}}{T^2}$$

θ = 548.68 K
C_1 = 302.27 J/kg-K
$C_2 = 8.463 \times 10^{-3}$ J/kg-K^2
$C_3 = 8.741 \times 10^{7}$ J/kg
E_a = 18531.7 K



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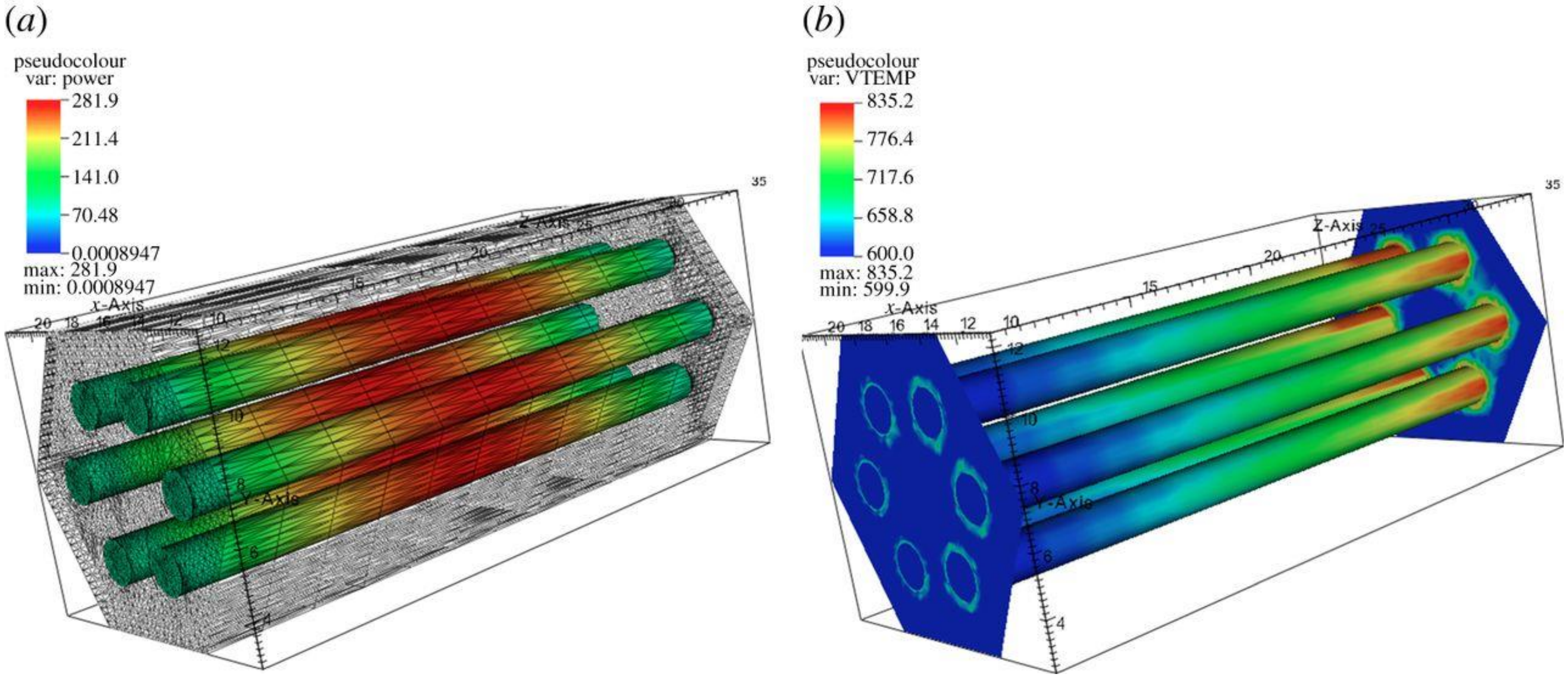
The heat generation rate is a function of the thermal neutron flux, which varies in time and space

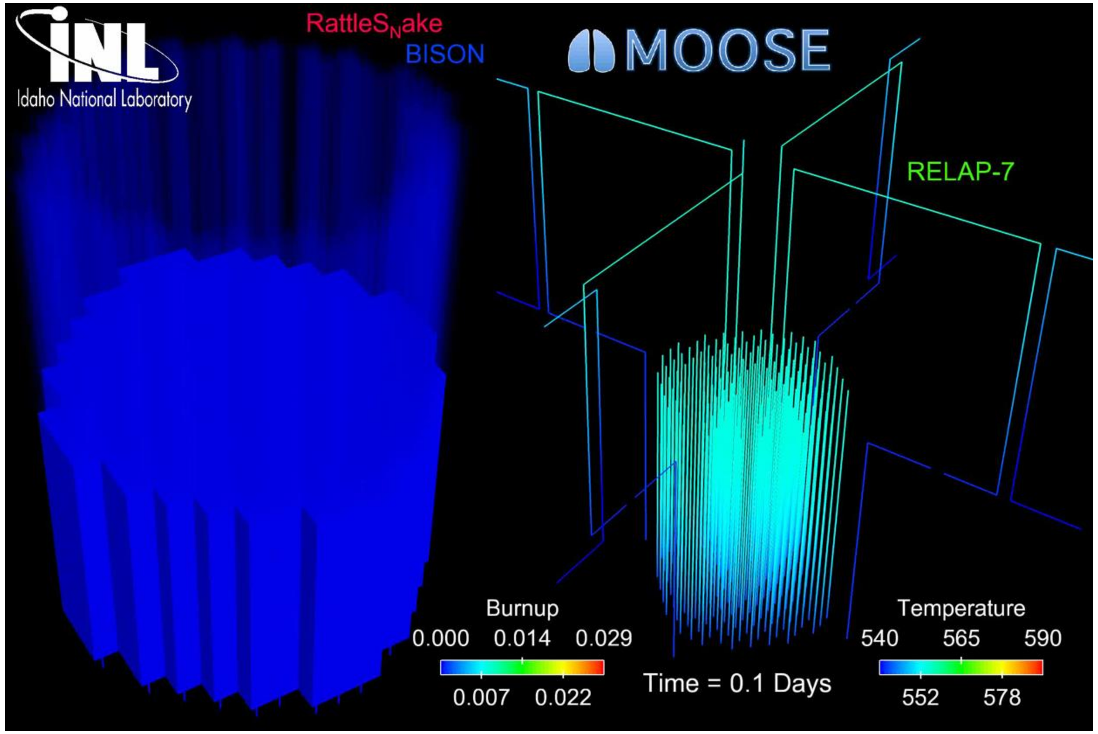
$$Q = E_f N_f \sigma_f \varphi_{th}$$



ANALYTICAL SOLVE OF HEAT CONDUCTION

The most accurate solution is numerical, in 3D, requires modeling the entire core, and is multi-physics

- Solution is 3D and changes in time
- All the properties are functions of temperature
- The boundary conditions comes from information about the coolant flow
- The heat generation rate comes from information about the neutronics in the reactor
- No analytical solution is possible



In order to solve, make assumptions!

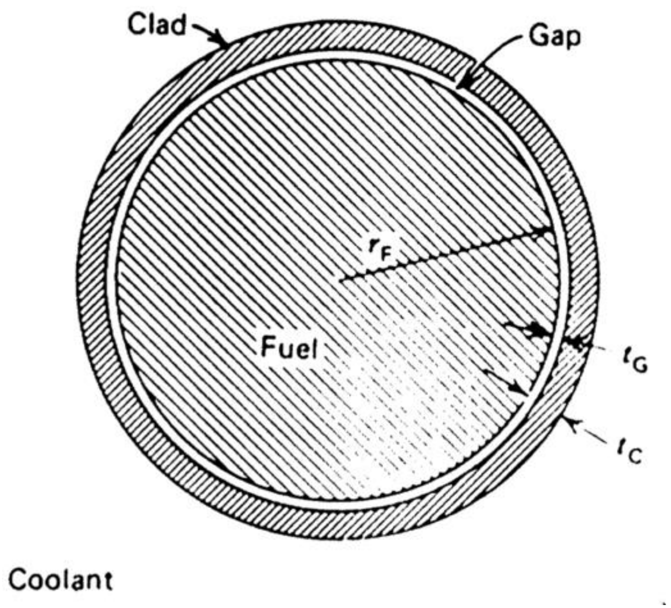
$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

- #1: steady state -> $\nabla \cdot (k \nabla T) + Q = 0$
- #2: cylindrical, axisymmetric ->

$$\frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k(T)\frac{\partial T}{\partial z}\right) + Q(r,z) = 0$$

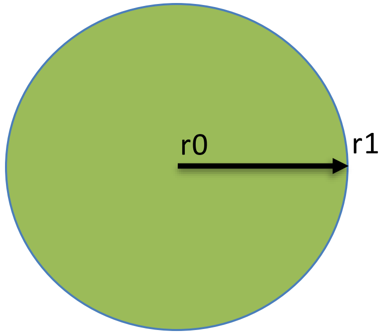
- #3: constant in z $\frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T}{\partial r}\right) + Q(r) = 0$
- #4: constant thermal conductivity, volume heat

$$\frac{1}{r}\frac{\partial}{\partial r}\left(rk\frac{\partial T}{\partial r}\right) + Q = 0$$



Directly Solving for Temperature Profile

- Boundary conditions: $r_0 = 0$, $r_1 = R$, $T'(0) = 0$, $T(R) = T_s$



$$\frac{1}{r}\frac{\partial}{\partial r}\left(rk\frac{\partial T}{\partial r}\right) + Q = 0$$

$$\frac{\partial}{\partial r}\left(rk\frac{\partial T}{\partial r}\right) = -Q\,r$$

$$rk\frac{\partial T}{\partial r} = -\frac{Q\,r^2}{2} + C_1 \qquad 0 = -\frac{Q\,0^2}{2} + C_1$$

$$\frac{\partial T}{\partial r} = -\frac{Q\,r}{2k}$$

$$T(r) = -\frac{Q\,r^2}{4k} + C_2 \qquad C_2 = \frac{QR^2}{4k} + T_s$$

$$T(r) = -\frac{Qr^2}{4k} + \frac{QR^2}{4k} + T_s \qquad T(r) = \frac{Q(R^2 - r^2)}{4k} + T_s$$

$$T_0 - T_s = \frac{QR^2}{4k}$$

Linear Heat Rate

- $LHR = \pi R^2 Q_{av}$
  - Where Q_{av} is the radially averaged heat generation rate in W/cm^3
  - LHR is in units of power per unit length: W/cm
- Substitute LHR into previous equation on T_0-T_s

$$T_0 - T_s = \frac{QR^2}{4k} \qquad T_0 - T_s = \frac{R^2}{4k}\frac{LHR}{\pi R^2} \qquad T_0 - T_s = \frac{LHR}{4\pi k}$$

Alternate Geometries

- Similar derivation with appropriate boundary conditions can be applied to plate and sphere geometries

Plate

$$T(x) - T_s = \frac{LHR}{2\pi k}\left(1 - \frac{x^2}{t_f^2}\right)$$

x is the distance from the midplane of the fuel and tf is the plate fuel thickness

Sphere

$$T(r) - T_s = \frac{LHR}{6\pi k}\left(1 - \frac{r^2}{R_f^2}\right)$$

r is the distance from the sphere center and Rf is the radius of the sphere

Heat transport through the gap

- Heat flux is a conserved quantity, described by Fourier's first and second laws:
- If there are no sources of heat, as if the case in the cladding and gap, the temperature field is constant with time, and the heat flux is unidirectional
- For boundary conditions T1 and T2 and a thickness d
- This assumes a spatially constant thermal conductivity, consistent with a "thin slab"

$$\vec{q} = -\lambda \nabla T ,$$

$$\rho c \frac{\partial T}{\partial t} = \nabla(\lambda \nabla T) + q^*,$$

λ = thermal cond.

$$q = -\lambda \frac{dT(x)}{dx},$$

$$q = \frac{T_1 - T_2}{\frac{d}{\lambda}} \qquad T(x) = T_1 - \frac{T_1 - T_2}{d} x$$

Heat transport through the gap

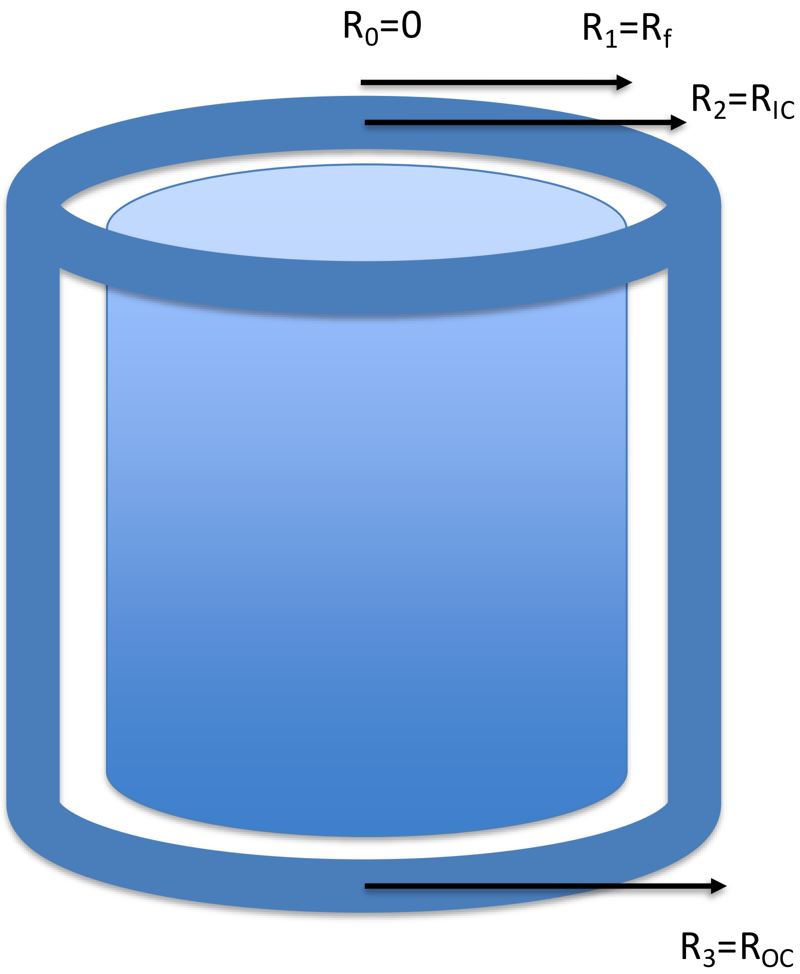
- The heat flux gives the rate, per unit area, at which heat flows in a given direction

$$q = -k\frac{T_2 - T_1}{d} \qquad q_{gap} = -k_{gap}\frac{T_{IC} - T_{fuel}}{R_{IC} - R_{fuel}}$$

- The heat flux from the fuel is the LHR/pellet circumference

$$q = \frac{LHR}{2\pi R_f}$$

- Heat flux from the fuel is the same as heat flux through the the gap – can make this assumption because $R_f >> t_g$
- Gap thickness = R_{IC}-R_f = t_g
- Cladding thickness = R_{OC}-R_{IC} = t_c



Heat transport through the gap

- Set heat flux fuel/gap equal

$$\frac{LHR}{2\pi R_f} = -k_{gap}\frac{T_{IC} - T_{fuel}}{t_{gap}} \qquad \frac{LHR}{2\pi R_f} = k_{gap}\frac{T_{fuel} - T_{IC}}{t_{gap}}$$

- Gap conductance is defined as:

$$h_g = \frac{k_{gap}}{t_g} \qquad T_{fuel} - T_{IC} = \frac{LHR}{2\pi R_f h_g}$$

- Gap conductance depends on the gas filling the gap
  - For pure He, $k_{gap}=16\text{x}10^{-6} * T^{0.79}$ (W/cm-K)
  - For pure Xe, $k_{gap}=0.7\text{x}10^{-6} * T^{0.79}$ (W/cm-K)
  - Simple mixing rule: $k_{gap} = k_{He}(1-y) + k_{Xe}y$
    - Where y is the mole/atom fraction of Xe

Heat transport through the cladding

- Heat flux through the cladding

$$q = -k\,\frac{T_2 - T_1}{d} \qquad q_{clad} = -k_{clad}\,\frac{T_{OC} - T_{IC}}{R_{OC} - R_{IC}}$$

$$q = \frac{LHR}{2\pi R_f} \qquad q_{clad} = k_{clad}\,\frac{T_{IC} - T_{OC}}{t_{clad}}$$

- Set equal your heat fluxes

$$\frac{LHR}{2\pi R_f} = k_{clad}\,\frac{T_{IC} - T_{OC}}{t_{clad}} \qquad T_{IC} - T_{OC} = \frac{LHR}{2\pi R_f}\frac{t_{clad}}{k_{clad}}$$

Heat transfer to the coolant

- Heat is transported from the cladding to the coolant via convection

$$T_{CO} - T_{cool} = \frac{LHR}{2\pi R_F h_{cool}}$$

- T_{cool} is the coolant temperature, h_{cool} is the convective heat transfer coefficient between cladding wall and coolant

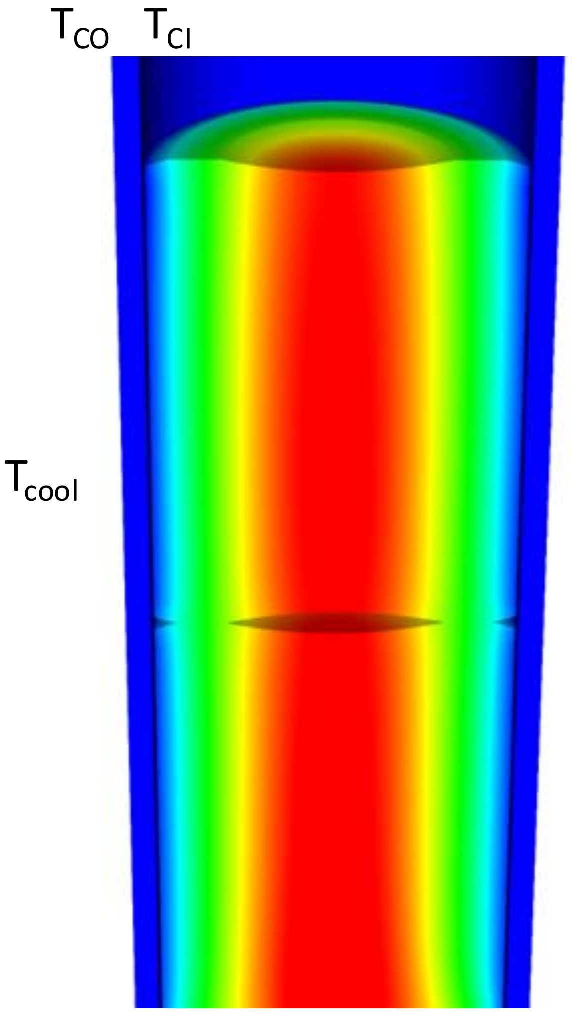
- Adding gap + cladding + coolant: $\frac{1}{h} = \frac{t_{gap}}{k_{gap}} + \frac{t_{clad}}{k_{clad}} + \frac{1}{h_{cool}}$

Summary of analytical solutions

- $T_0 - T_{fuel} = \frac{Q}{4k} R_{fuel}^2$ $\quad T_0 - T_{fuel} = \frac{LHR}{4\pi k}$
- $T_{fuel} - T_{IC} = \frac{Q}{2h_{gap}} R_{fuel}$ $\quad T_{fuel} - T_{IC} = \frac{LHR}{2\pi R_{fuel} h_{gap}}$ $\quad h_{gap} = \frac{k_{gap}}{t_{gap}}$
- $T_{IC} - T_{OC} = \frac{Q t_{clad}}{2k_{clad}} R_{fuel}$ $\quad T_{IC} - T_{OC} = \frac{LHR\, t_{clad}}{2\pi R_{fuel} k_{clad}}$
- $T_{OC} - T_{cool} = \frac{Q}{2h_{cool}} R_{fuel}$ $\quad T_{OC} - T_{cool} = \frac{LHR}{2\pi R_{fuel} h_{cool}}$

Solving for the temperature profile

- You solve for the transition temperatures
- Start from the coolant (known BC) and work inward
- Have a linear profile everywhere except in the fuel
- Finally, solve for the temperature profile throughout the fuel



Fuel and Cladding Thermal Properties

Material	Density (g/cm^3)	Heat Capacity Cp (J/g-K)	Thermal Conductivity k (W/cm-K)	Thermal Expansion Coefficient a (K^{-1})
UO_2	10.98	0.33	0.03	1.2 x 10^{-5}
Zr	6.5	0.35	0.17	1.0 x 10^{-5}
Stainless steel	8.0	0.5	0.17	9.6 x 10^{-6}

Example Problem

Temperature profile calculation example

- **T_{cool} = 580 K; LHR = 200 W/cm; h_{cool} = 2.65 W/cm^2-K**
- **R_{fuel} = 0.5 cm; t_{clad} = 0.06 cm; t_{gap} = 0.003 cm; k_f=0.03 W/cm-K**
- Work from outside->in, calculate cladding temperature

  T_{co} = (200)/(2*pi*0.5*2.65) + 580

  $$T_{co} - T_{cool} = \frac{LHR}{2\pi R_{fuel} h_{cool}}$$

  T_{co} = 604 K
- Calculate inner cladding temp

  T_{ci} = (200*0.06)/(2*pi*0.5*0.17) + 604

  $$T_{ci} - T_{clad} = \frac{LHR\, t_{clad}}{2\pi R_{fuel} k_{clad}}$$

  T_{ci} = 626 K

Temperature profile calculation example

- Calculate fuel surface temperature
- Calculate gap conductance
  - gap with He; k_{gap}=16x10^{-6} * T$^{0.79}$ (W/cm-k); assume T_{ci} is appropriate for entire gap; k_{gap} = 0.0026 W/cm-K; t_{gap} = 0.003 cm
  - h_{gap} = 0.87 W/cm^2-K

T_{fuel} = 200/(2*pi*0.5*0.87) + 626.5

$$T_{fuel} - T_{ci} = \frac{LHR}{2\pi R_{fuel} h_{gap}}$$

T_{fuel} = 700.3 K

Temperature profile calculation example

- Calculate centerline temperature

T_0 = 200/(4*pi*0.03) + 700.3

T_0 = 1230.8 K

$$T_0 - T_{fuel} = \frac{LHR}{4\pi k}$$

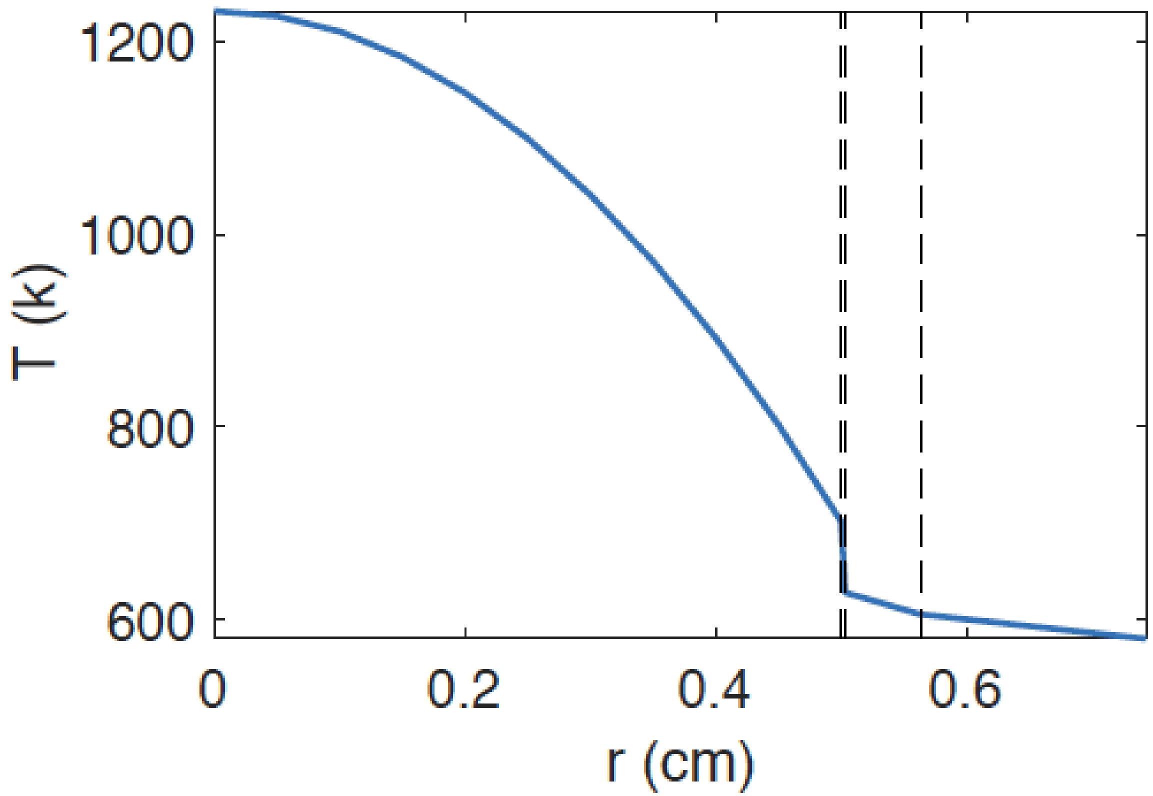
Full temperature profile

$$T(r) = \frac{Q(R^2 - r^2)}{4k} + T_s$$

$$T(r) = \frac{LHR(R_f^2 - r^2)}{4\pi k R_f} + T_s \qquad T(r) = \frac{LHR}{4\pi k}\left(1 - \frac{r^2}{R_f^2}\right) + T_s$$

Temperature profile calculation example

- Parabolic temperature profile in fuel
- Linear in gap and clad
- Steep temperature drop over gap, very low thermal conductivity
- Smaller temperature drop over cladding



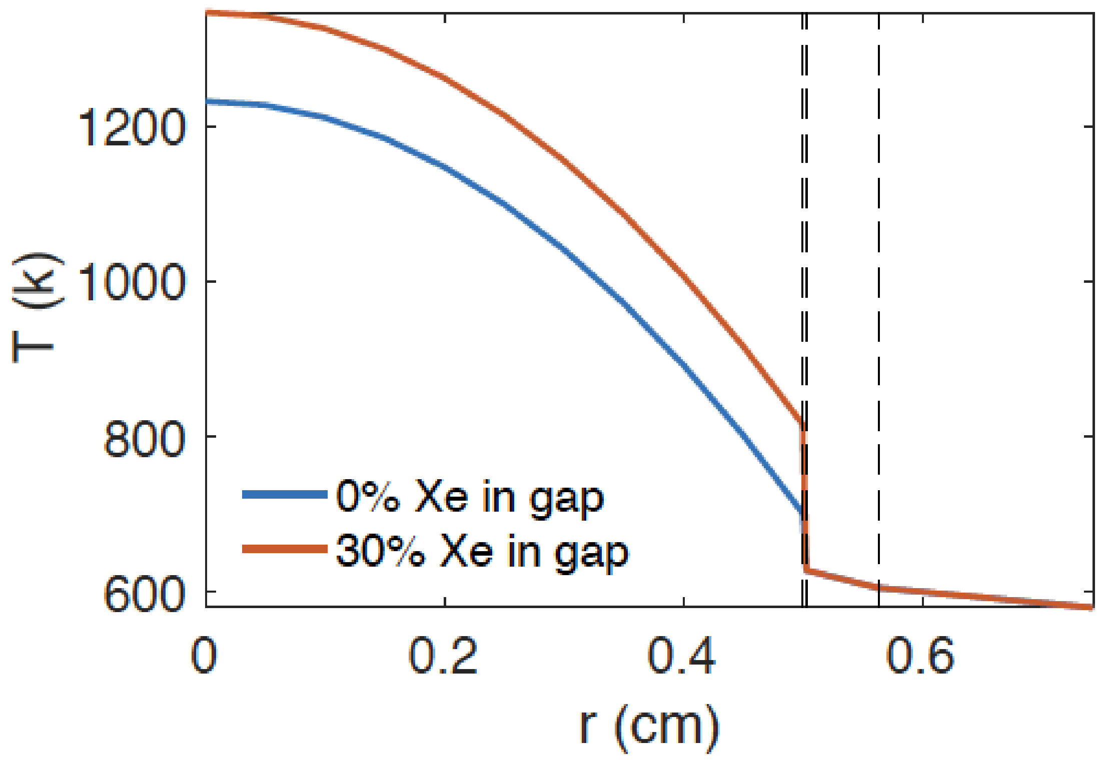
Temperature profile modification

- Instead of pure He gap, 30% of gas is Xe; how is T_0 affected?
- First, how is gap conductance affected?
- Gap conductance depends on the gas filling the gap
  - For pure He, $k_{gap}=16x10^{-6} * T^{0.79}$ (W/cm-K)
  - For pure Xe, $k_{gap}=0.7x10^{-6} * T^{0.79}$ (W/cm-K)
  - Simple mixing rule: $k_{gap} = k_{He}(1-y) + k_{Xe}y$
  - T_{Cl}, T_{CO}, and T_{cool} is unchanged from previous example, also T_0-T_{fuel} is unchanged
  - $k_{gap} = ((16x10^{-6})*(626)^{0.79})(1-0.3) + ((0.7x10^{-6})*(626)^{0.79})(0.3) = 1.85E-3$ W/cm-K

Temperature profile modification

- k_{gap} = 1.85E-3 W/cm-K
- h_{gap} = 1.85E-3 / 0.003 = 0.62 W/cm^2-K
- T_{fuel} = 200/(2*pi*0.5*0.62) + 626 = 729 K
- $T_0 - T_{fuel}$ = 530.5 K (unchanged from before)
- T_0 = 729 + 530.5 = 1259.5 K

- Increase in T_0 of 30 K
- Caveat: linear mixing of gases is not the best approach

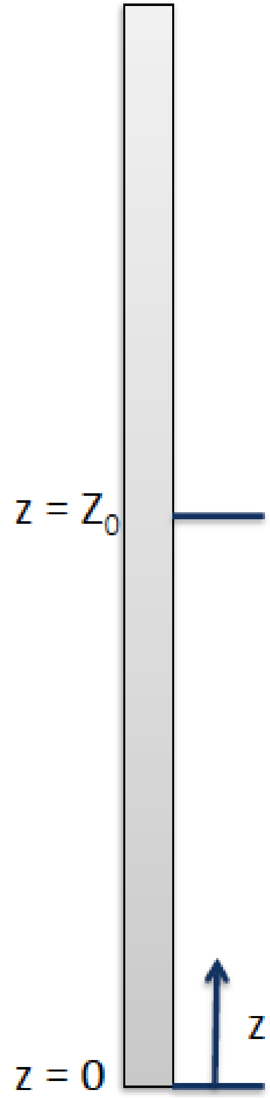


Neutron flux varies axially, so does LHR

- Taking a fuel rod with length, L = 2*Z_0

$$LHR\left(\frac{z}{Z_o}\right) = LHR^o \cos\left[\frac{\pi}{2\gamma}\left(\frac{z}{Z_o} - 1\right)\right] = LHR^o\, F\left(\frac{z}{Z_o}\right)$$

- LHR^0 is the midpoint linear heat rate, i.e. @ z=Z_0
- $\gamma = \frac{Z_{ex}+Z_0}{Z_0}$, where Z_{ex} is the extrapolation distance
- A typical value is $\gamma = 1.3$; can reduce $\pi/2\gamma$ to 1.2



Coolant temperature varies with Z

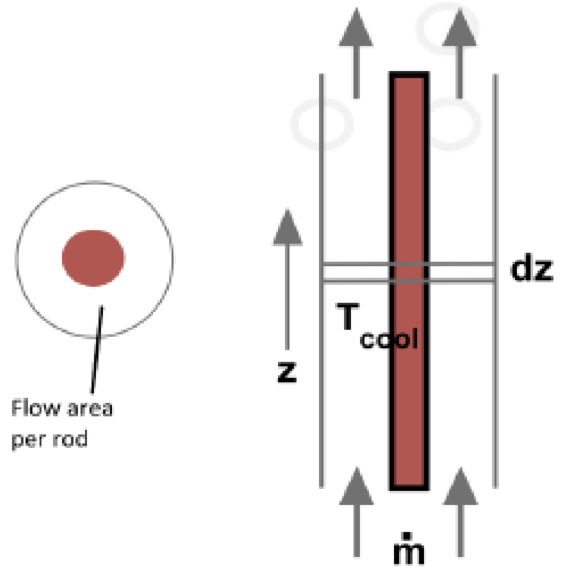
- Each rod has a given flow area
- Mass flow rate: $\dot{m}$
- Coolant specific heat: C_{PW}

$$\dot{m}C_{PW}\frac{dT_{cool}}{dz} = LHR\left(\frac{z}{Z_o}\right)$$

$$\dot{m}C_{PW}(T_{cool} - T_{cool}^{in}) = Z_o \int_0^{z/Z_o} LHR\left(\frac{z}{Z_o}\right) d\left(\frac{z}{Z_o}\right)$$

$$\dot{m}C_{PW}(T_{cool} - T_{cool}^{in}) = Z_o \times LHR^o \int_0^{z/Z_o} F\left(\frac{z}{Z_o}\right) d\left(\frac{z}{Z_o}\right)$$

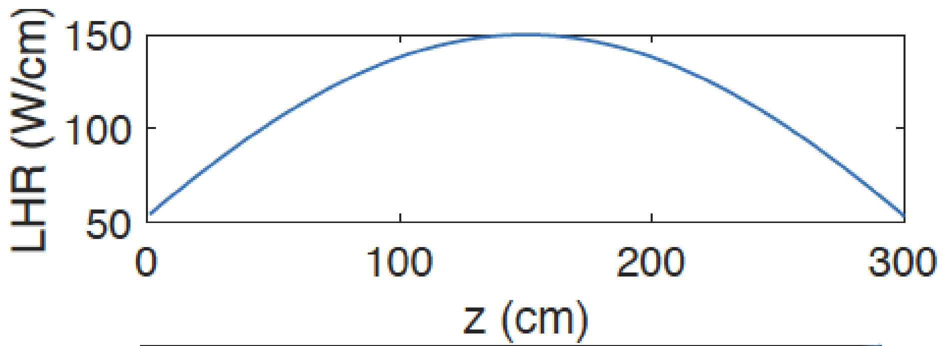
$$T_{cool} - T_{cool}^{in} = \frac{1}{1.2}\frac{Z_o \times LHR^o}{\dot{m}C_{PW}}\left\{\sin(1.2) + \sin\left[1.2\left(\frac{z}{Z_o} - 1\right)\right]\right\}$$

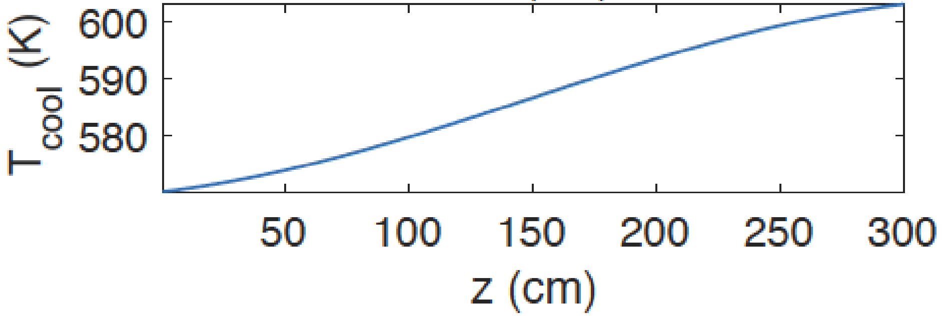


Calculate LHR and T_{cool} with axial variation

- mdot = 0.25 kg/s-rod; Z_0 = 150 cm; LHR^0 = 150 W/cm; C_{PW} = 4200 J/kg-K; T_{in}= 570 K

$$T_{cool} - T_{cool}^{in} = \frac{1}{1.2}\frac{Z_o \times LHR^o}{\dot{m} C_{PW}}\left\{\sin(1.2) + \sin\left[1.2\left(\frac{z}{Z_o} - 1\right)\right]\right\}$$





Summary

- Developed analytical expressions for the temperature profile within a fuel rod
- Required to make four assumptions:
  - Steady-state solution
  - Temperature is axisymmetric
  - T is constant in Z
  - Thermal conductivity is independent of temperature
- Temperature profile in the fuel is parabolic, assume linear profiles in gap, clad and coolant
- Can incorporate axial variation in T_{cool} with axial variation in LHR