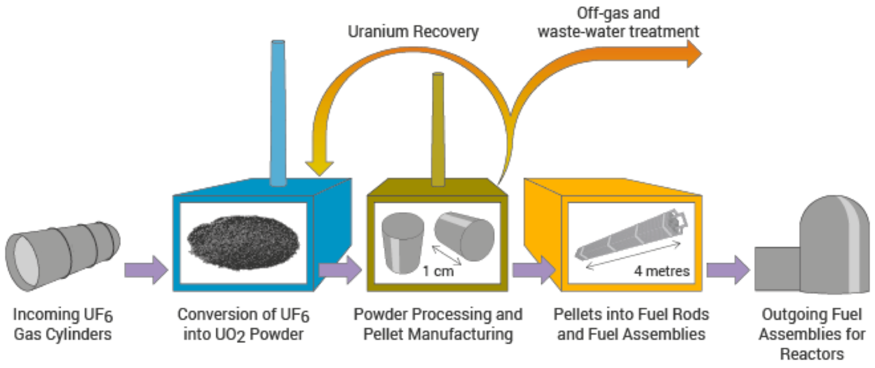
Nuclear Fuel Performance

NE 591

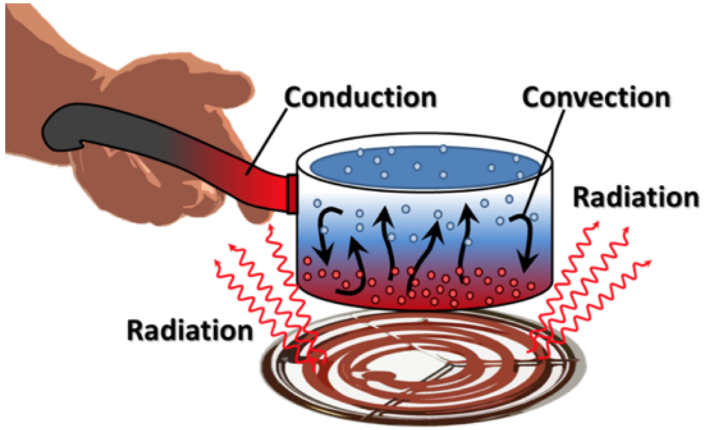
Last Time

- 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
- For different fuel types, enriched UF_6 follows a different path



Last Time

- General heat transport
- Heat is produced in the fuel, transports through the gap and cladding, and into the coolant
- The geometry of our problem
- The initial condition of T
- The boundary conditions of T
- Is each parameter is a function of T
  - Thermal conductivity, heat capacity
- Function of space/time?
  - Heat generation, dependent upon flux

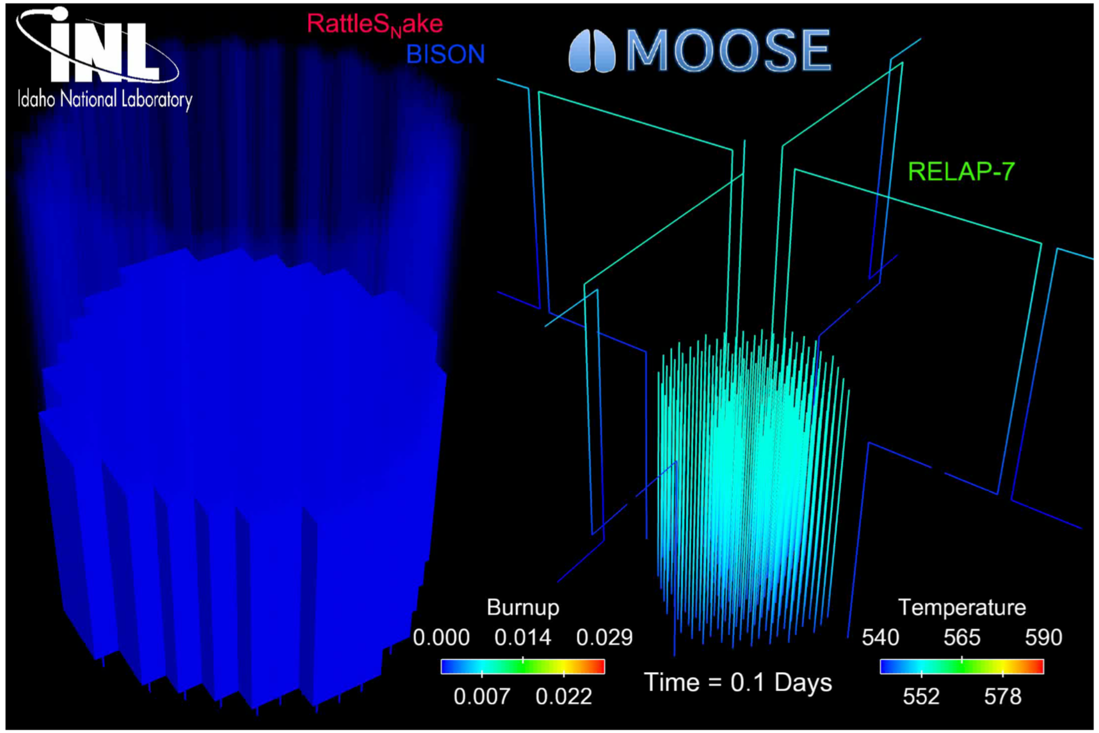


$$\rho c_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T)$$

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!

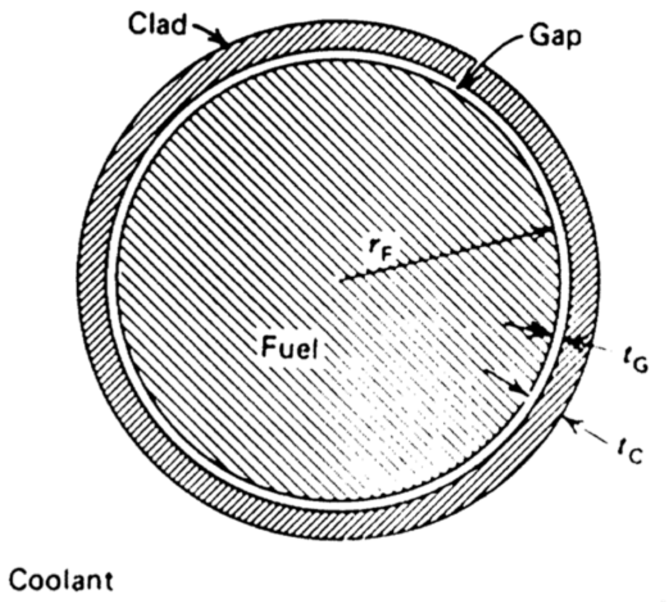
$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

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

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

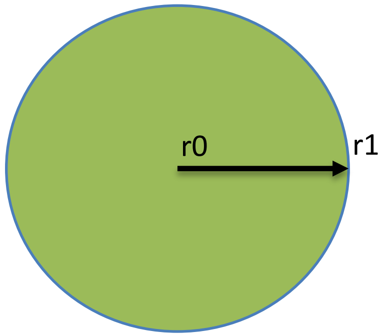
- #3: constant in z $\frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T}{\partial r}\right) + Q(r) = 0$
- #4: constant thermal conductivity

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



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 units of per-length, i.e. W/cm
- Substitute LHR into previous equation on T0-Ts

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

Heat transport through the gap

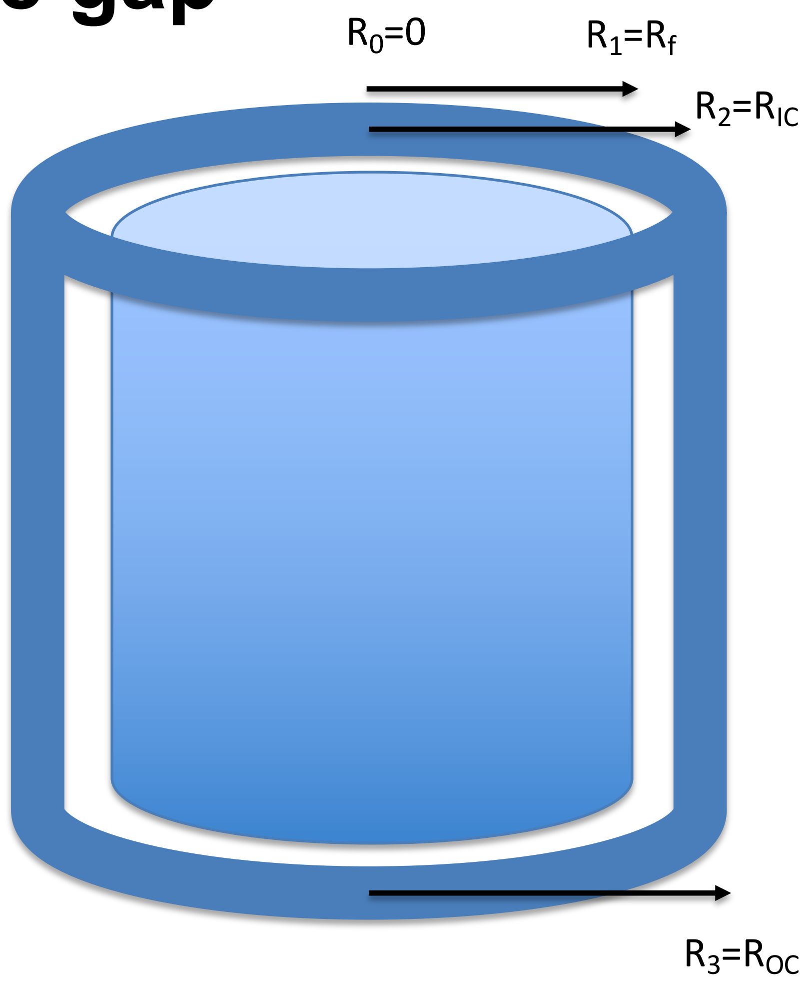
- The heat flux gives the rate, per unit area, at which heat flows in a given direction

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

- 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 into the gap
- 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

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

- Gap conductance is defined as:

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

- 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

$$q = -k\frac{T_2 - T_1}{L} \qquad q_{clad} = -k_{clad}\frac{T_{co} - T_{ci}}{R_{co} - R_{ci}}$$

$$q = \frac{LHR}{2\pi R_f} \qquad q_{clad} = k_{clad}\frac{T_{ci} - T_{co}}{t_{clad}}$$

- Set equal your heat fluxes

$$\frac{LHR}{2\pi R_f} = k_{clad}\frac{T_{ci} - T_{co}}{t_{clad}} \qquad T_{ci} - T_{co} = \frac{LHR}{2\pi R_f}\frac{t_{clad}}{k_{clad}}$$

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

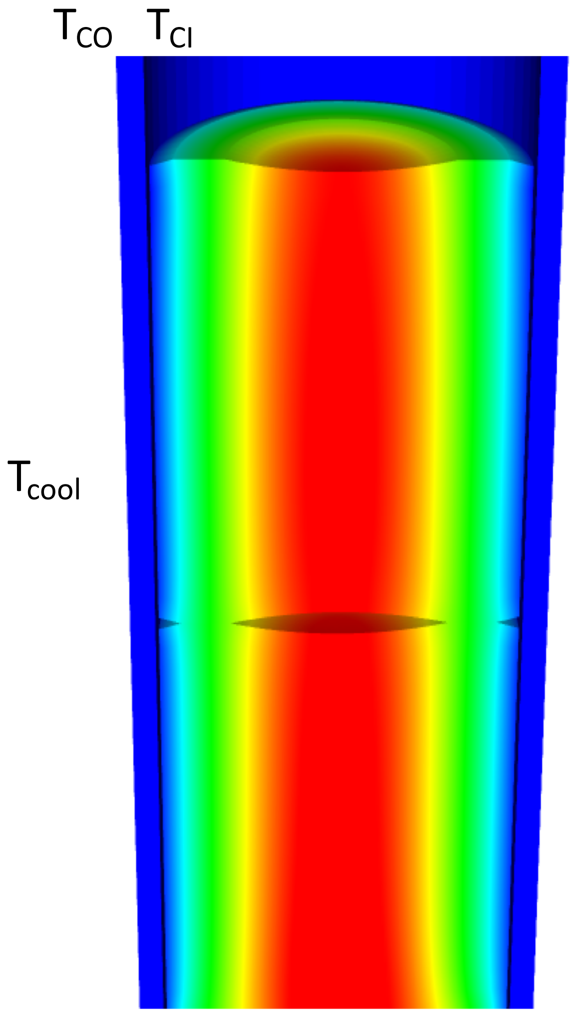
- Adding gap + cladding + coolant: $\frac{1}{h} = \frac{t_{gap}}{k_{gap}} + \frac{t_{clad}}{k_{clad}} + \frac{1}{h_{cool}}$

Summary of analytical solutions

- $T_0 - T_{fuel} = \frac{Q}{4k} R_{fuel}^2$ $\qquad$ $T_0 - T_{fuel} = \frac{LHR}{4\pi k}$
- $T_{fuel} - T_{gap} = \frac{Q}{2h_{gap}} R_{fuel}$ $\qquad$ $T_{fuel} - T_{gap} = \frac{LHR}{2\pi R_{fuel} h_{gap}}$ $\qquad$ $h_{gap} = \frac{k_{gap}}{t_{gap}}$
- $T_{gap} - T_{clad} = \frac{Qt_{clad}}{2k_{clad}} R_{fuel}$ $\qquad$ $T_{gap} - T_{clad} = \frac{LHRt_{clad}}{2\pi R_{fuel} k_{clad}}$ $\qquad$ T_{gap} = T_{CI} (clad inner)
T_{clad} = T_{CO} (clad outer)
- $T_{clad} - T_{cool} = \frac{Q}{2h_{cool}} R_{fuel}$ $\qquad$ $T_{clad} - T_{cool} = \frac{LHR}{2\pi R_{fuel} h_{cool}}$

Solving for the temperature profile

- You first solve for the transition temperatures.
- Start from the coolant and work inward
- Then, assume 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	1.2×10^{-5}
Zr	6.5	0.35	0.17	1.0×10^{-5}
Stainless steel	8.0	0.5	0.17	9.6×10^{-6}

Temperature profile calculation example

- **T_{cool} = 580 K; LHR = 200 W/cm; h_{cool} = 2.5 W/cm^2-K**
- **R_{fuel} = 0.5 cm; t_{clad} = 0.06 cm; t_{gap} = 0.003 cm**
- Work from outside->in, calculate cladding temperature

T_{co} = (200)/(2*pi*0.5*2.5) + 580

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

T_{co} = 605.5 K

- Calculate inner cladding temp

T_{ci} = (200*0.06)/(2*pi*0.5*0.17) + 605.5

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

T_{ci} = 628 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) + 628

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

T_{fuel} = 701.5 K

Temperature profile calculation example

- Calculate centerline temperature

T_0 = 200/(4*pi*0.03) + 701.5

T_0 = 1232 K

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

Full temperature profile

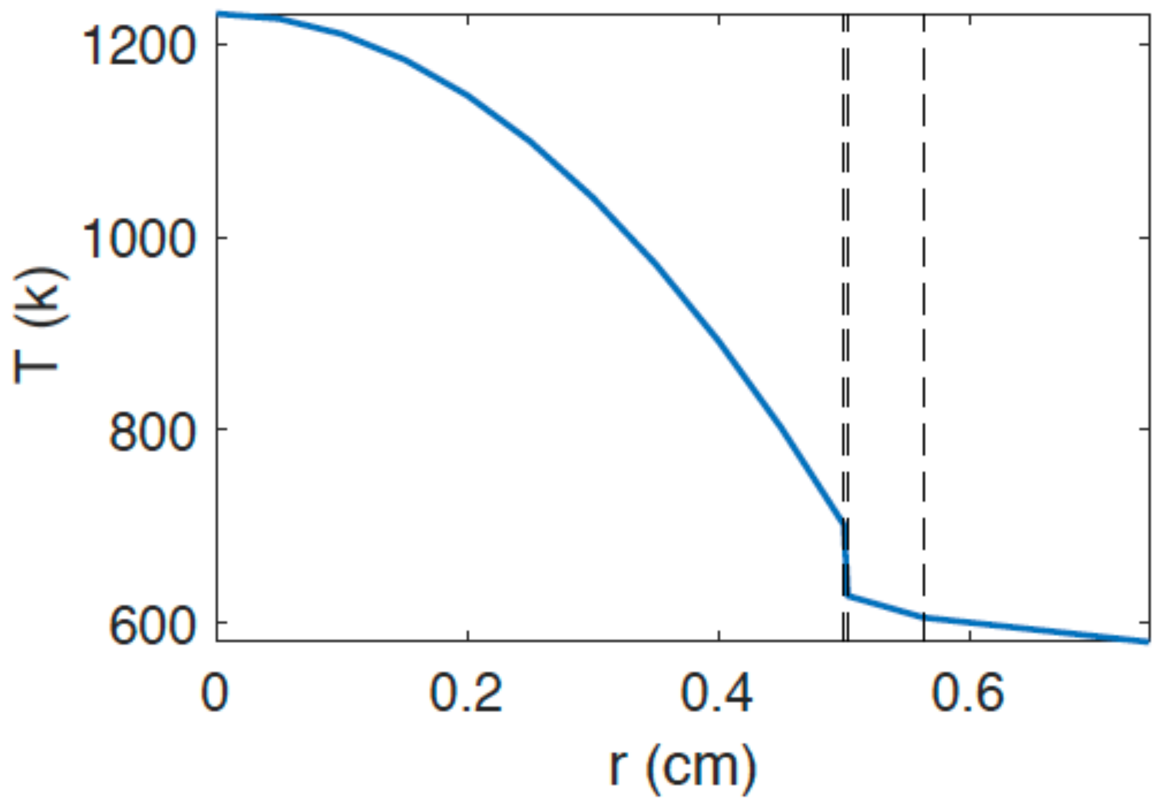
$$T(r) = \frac{Q(R^2 - r^2)}{4k} + T_s$$

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

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

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



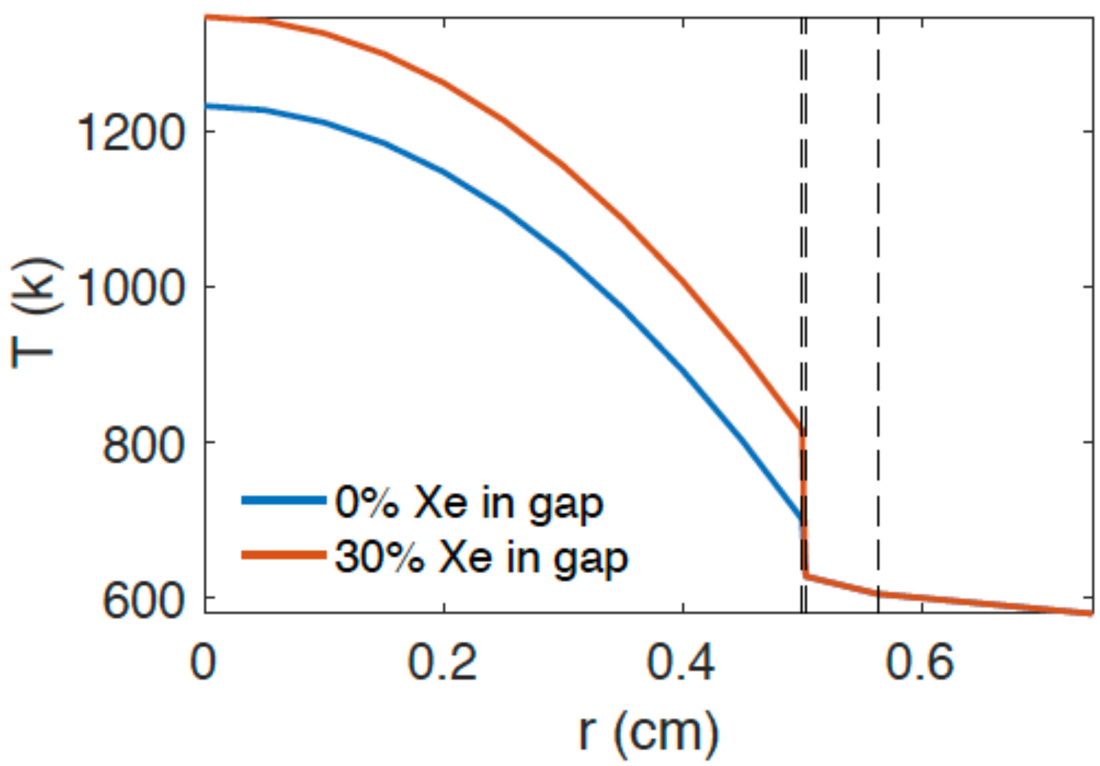
Temperature profile modification

- 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, $k_{gap}=16\text{x}10^{-6} * T^{0.79}$ (W/cm-K)
  - For pure Xe, $k_{gap}=0.7\text{x}10^{-6} * T^{0.79}$ (W/cm-K)
  - Simple mixing rule: $k_{gap} = k_{He}(1\text{-}y) + k_{Xe}y$
  - T_{CI}, T_{CO}, and T_{cool} is unchanged from previous example, also $T_0\text{-}T_{fuel}$ is unchanged
  - $k_{gap} = ((16\text{x}10^{-6})*(628)^{0.79})(1\text{-}0.3) + ((0.7\text{x}10^{-6})*(628)^{0.79})(0.3) = 1.85\text{E-}3$ 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) + 628 = 731 K
- $T_0 - T_{fuel}$ = 530.5 K (unchanged from before)
- T_0 = 731 + 530.5 = 1261.6 K

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

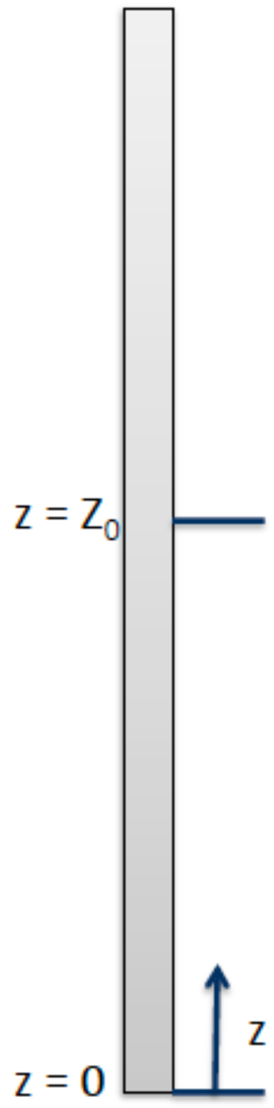


Neutron flux varies axially, so does LHR

- 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 $\gamma = 1.3$



Coolant temperature varies with Z

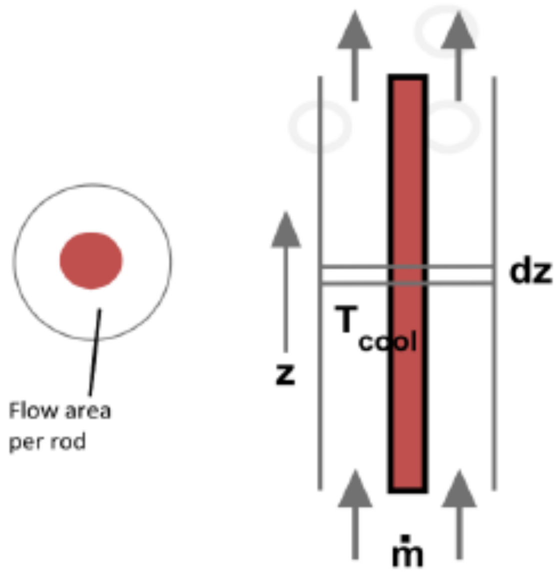
- Each rod has a given flow area
- Mass flow rate: $\dot{m}$
- Coolant specific heat: C_{PW}

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

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

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

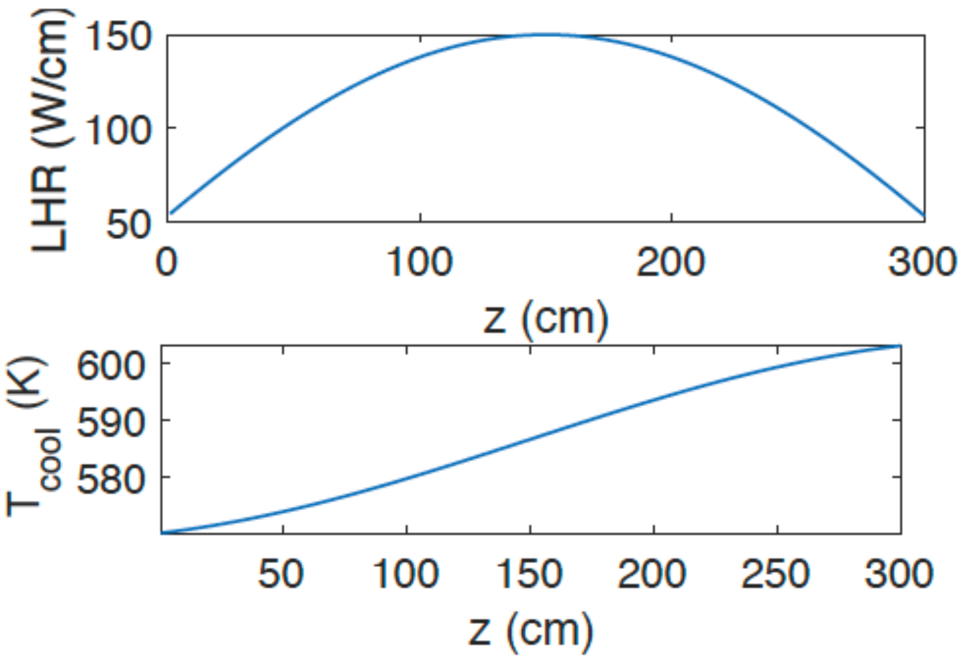
$$T_{cool}-T_{cool}^{in}=\frac{1}{1.2}\frac{Z_o\times LHR^o}{\dot{m}C_{PW}}\left\{\sin(1.2)+\sin\left[1.2\left(\frac{z}{Z_o}-1\right)\right]\right\}$$



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

NUMERICAL TIME INTEGRATION

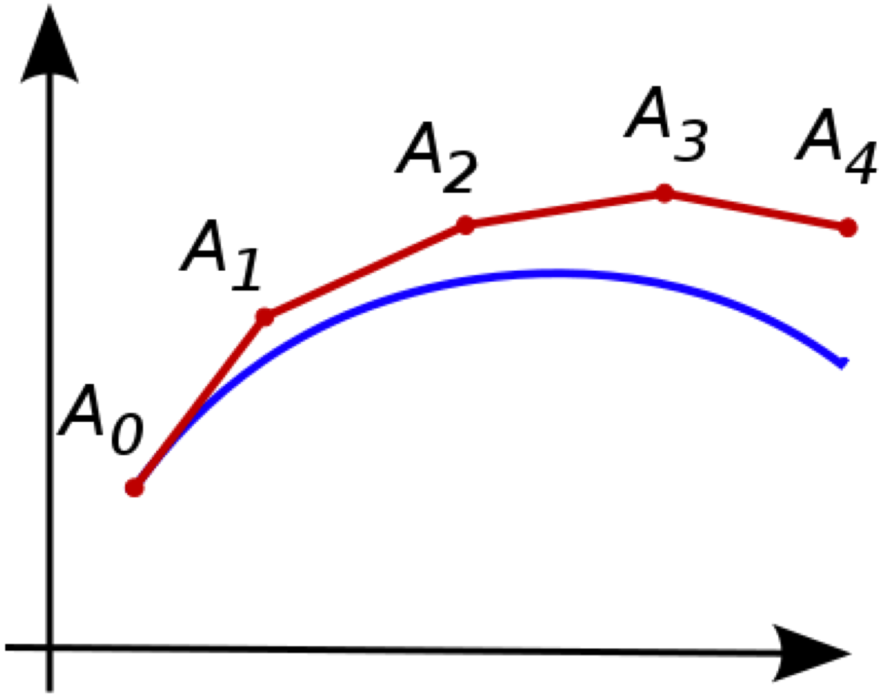
For numerical solutions, deal with derivatives in space/time

- Derivatives in time
  - Forward Euler’s method (explicit)
  - Backward Euler’s method (implicit)
- Derivatives in space
  - Finite difference
  - Finite volume
  - Finite element

Forward Euler

- Step forward through time in increments, dt
- The Euler method is a first-order method, which means that the local error (error per step) is proportional to the square of the step size
- Expand a function y(t), with a timestep size, h

  $$y(t_0 + h) = y(t_0) + h\,y'(t_0) + \frac{1}{2}h^2 y''(t_0) + \cdots$$
- Euler takes only the first derivative
- $y_{n+1} = y_n + hy'(t)$
- Value y_n is an approximation of the solution to the ODE at time t_n



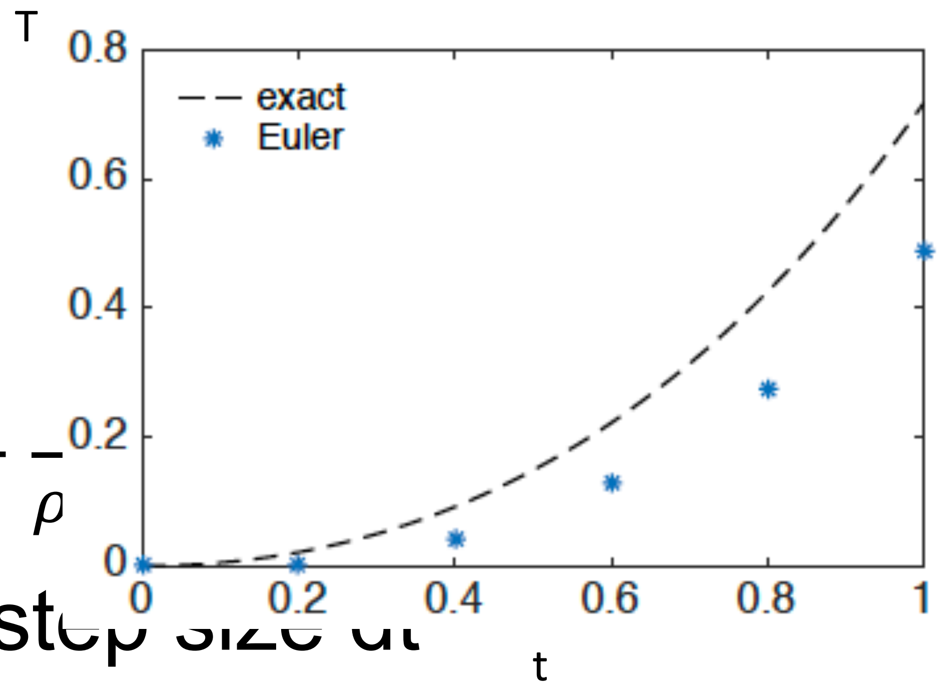
Forward Euler

- Applying to our temperature system

$$T(r,t+dt) = T(r,t) + dt\,\frac{\partial T(r,t)}{\partial t}$$

- Using the heat conduction equation:

$$\frac{\partial T(r,t)}{\partial t} = \frac{1}{\rho c_p}\frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T(r,t)}{\partial t}\right) + \frac{}{\rho}$$



- We input T_0, which here is T @ t=0, step size dt

$$T_{n+1} = T_n + dt^*T'; \; t_{n+1} = t_n + dt$$

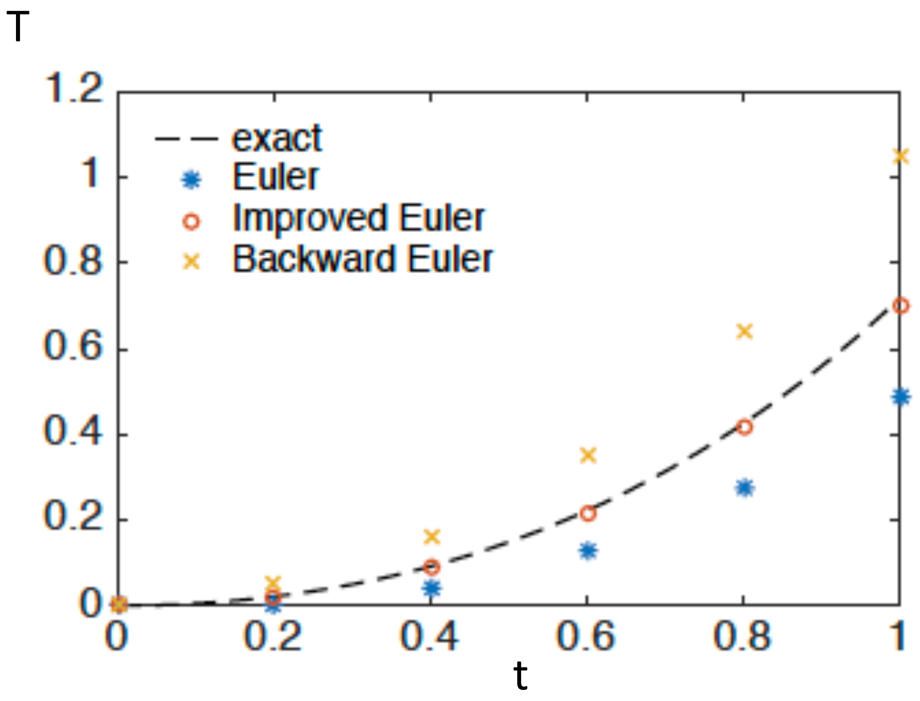
Backwards Euler

- Backwards Euler for a function T(r,t)

$$T(r,t+dt) = T(r,t) + dt\frac{\partial T(r,t+dt)}{\partial r}$$

$$\frac{\partial T(r,t+dt)}{\partial r} = \frac{1}{\rho c_p}\frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T(r,t+dt)}{\partial r}\right) + \frac{1}{\rho c_p}Q(r)$$

- This differs from Forward Euler in that here we use (r,t+dt), instead of (r,t)
- $T_{n+1} = T_n + dt\, T'(r,t+dt)$, $t_{n+1} = t_n + dt$
- The new approximation appears on both sides of the equation, thus this method needs to solve an algebraic equation for the unknown future state
- This can be done with fixed-point iteration or non-linear solvers
- Improved Euler is a form of explicit Euler (explicit trapezoidal rule), which takes the derivative at the midpoint



Explicit vs Implicit

- Forward Euler is explicit
  - Explicit methods calculate the state of a system at a later time from the state of the system at the current time
  - Can be unstable if step size is too much
- Backwards Euler is implicit
  - Implicit methods find a solution by solving an equation involving both the current state of the system and a later state
  - Implicit require an extra computation and they can be much harder to implement
  - Implicit methods are used because many problems arising in practice are stiff, for which the use of an explicit method requires very small timesteps