# Fundamentals of Nuclear Engineering

Module 6: *Neutron Diffusion*

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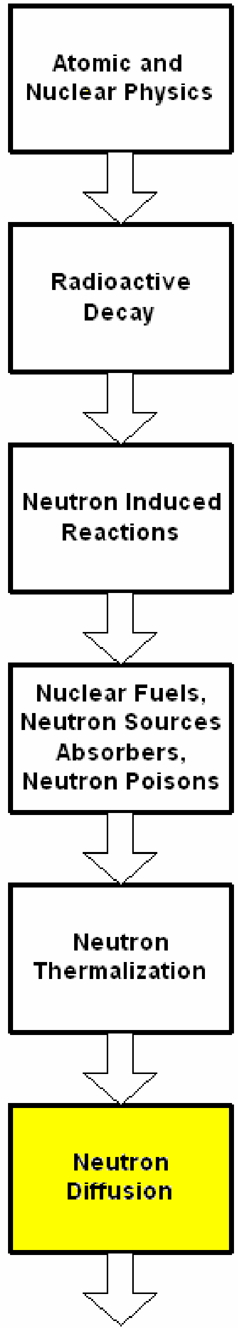



Basics of Atomic vs. Nuclear structure, definitions of terms used in future modules

Describes radioactive decay processes, half-life vs. decay rate used in future modules

Describes concept of cross sections, neutron induced reaction rates

Describes fissionable fuels, neutron sources, absorber materials, and fission product poisons impacting chain reactions

Describes process of neutron moderation used in thermal reactors, identifies impact of resonance capture which impacts chain reactions

Describes neutron diffusion model used to analyze chain reactions and other future reactor problems

# *Objectives:*

1. Understand how Neutron Diffusion explains reactor neutron flux distribution
2. Understand origin, limitations of Neutron Diffusion from:
    - Boltzmann Transport Equation,
    - Ficke's Law
3. Solution of One-Group Neutron Diffusion Equation for:
    - Cubical,
    - Cylindrical geometries (via separation of variables technique)
4. Identify Eigenvalues of Neutron Diffusion Equation (Buckling, Diffusion Length) related to physical properties
5. Understand refinements from Multi-Group Diffusion Model applied to Reflectors, flux depression near strong neutron absorbers, and sources

# *Boltzmann's Transport Equation*

- Originates from *Statistical Mechanics*
- Used to understand kinetic theory of gasses
- Full equation expressed as integral-differential equation
- In simplest terms it is a *conservation equation*

$$\frac{d}{dt}\int_V N(r,v,t)d^3r = \int_V S(r,t)d^3r - \int_V N(r,v,t)v\Sigma_c(r,v,t)d^3r - \oint \vec{J}(r,v,t)\bullet \vec{n}dA$$

Local Rate of Change in average Neutron Density

Local Rate of Neutrons added by Source

Local Rate of Neutrons Captured

Local Rate of Neutrons Streaming out of Local Volume

# *Boltzmann's Transport Equation*

- First simplification: *Apply Divergence Theorem*

$$\oint \vec{J}(r,v,t) \bullet \vec{n} dA = \int_V \vec{\nabla} \bullet \vec{J}(r,v,t) d^3 r$$

- Remove volume integration:

$$\frac{d}{dt} N(r,v,t) = S(r,t) - N(r,v,t) v \Sigma_c (r,v,t) - \vec{\nabla} \bullet \vec{J}(r,v,t)$$

- Divergence of Local Neutron Current is simplified by making "Diffusion Approximation"
- Alternate solution approach is via Monte Carlo Method
- Diffusion Approximation is based upon *Fick's Law*

# *Diffusion Approximation Assumes:*

- Uniform relatively infinite medium thus: $\Sigma_c(r) \sim \Sigma_c$
- No strong "point" neutron sources in medium
- Scattering collisions in Laboratory Frame of Reference are isotropic, thus: $d\sigma_s/d\Omega \sim \sigma_s/4\pi$
- Neutron flux $\Phi(r)$ is slowly varying function of position (no discontinuities, small $d\Phi/dr$ and higher terms)
- Neutron flux $\Phi(r)$ is independent of time

# *Diffusion Approximation to Neutron Transport*

- Expression for neutron streaming loss becomes

$$\vec{\nabla} \bullet \vec{J} = -\frac{\Sigma_s}{3\Sigma_t^{\ 2}} \vec{\nabla} \bullet \overrightarrow{\nabla}\phi = -\frac{\Sigma_s}{3\Sigma_t^{\ 2}} \nabla^2 \phi = -D\nabla^2 \phi$$

- Term: $\Sigma_s / 3\Sigma_t^2 = D$ - diffusion coefficient – *assumed to be spatially constant*

- Common approximation: $D \sim 1/ [3\ \Sigma_s(1- 2/3A)]$

- Neutron transport equation becomes:

$$\frac{dN(r)}{dt} = S(r) - N(r)v\Sigma_c(r) + D\nabla^2\phi(r)$$
$$= S(r) - \phi(r)\Sigma_c(r) + D\nabla^2\phi(r)$$

# *Diffusion Approximation to Neutron Transport*

- Neutrons are mono energetic and physical properties are averages

- $D(E) \sim D$ - for *some energy range*

- $\Sigma_t(E) \sim \Sigma_t$ - for *some energy range*

- $\Sigma_c(E) \sim \Sigma_c$ - for *some energy range*

# *What is Meant for: "some energy range"*

- From previous lectures:
- Effect of resonance scattering and absorption we know is *complex*
- Using "single values" to represent $\Sigma_s(E)$ *or* $\Sigma_c(E)$ is hard to believe
- Once neutrons pile up in thermal region use of thermal averaged values would seem reasonable
- Analytical technique is to break up energy spectrum into numerous energy groups and compute average values of key parameters
- As an example an averaged capture cross section for energies between $E_i$ and $E_j$ would be:

$$\Sigma_{c,ij} = \frac{\int_{E_i}^{E_j} \phi(E)\Sigma_c(E)dE}{\int_{E_i}^{E_j} \phi(E)dE}$$

- This implies *multiple one-speed diffusion equations,* with *multiple constants*

# *Steady State Neutron Diffusion*

- In steady state, diffusion equation is balance between source (+) vs. capture and diffusion (-)

$$S(r) = \phi(r)\Sigma_c(r) - D\nabla^2\phi(r)$$

- Types of neutron sources $S(r)$ could be:
- $(\alpha,n)$ reaction type source ($Pu$-$Be$, or $Am$-$Be$)
- Neutrons produced via $(n,f)$ chain fission reaction and thus proportional to flux: $\Phi(r)$

$$S(r) = \Sigma_c(r)\, k\, \Phi(r)$$

- *- where "$k$" is multiplication factor*
- *More to come on multiplication factors - <u>later</u>*

# *Diffusion from Point Neutron Source*

- In spherical geometry, Laplacian operator becomes:

$$\nabla^2 \phi(r) = \frac{d^2\phi(r)}{dr^2} + \frac{2}{r}\frac{d\phi(r)}{dr}$$

- Diffusion equation becomes after rearranging:

$$\frac{d^2\phi(r)}{dr^2} + \frac{2}{r}\frac{d\phi(r)}{dr} - \frac{\Sigma_c}{D}\phi(r) = -\frac{S_o}{D}$$

- Making change of variables: $y(r) = r\,\Phi(r)$, above expression simplifies to:

$$\frac{d^2 y(r)}{dr^2} - \frac{\Sigma_c}{D} y(r) = -\frac{S_o}{D}$$

# *Diffusion from Point Neutron Source*

- Solution: Define $L^2 = D / \Sigma_c$ - then $y(r) = A\, e^{-r/L} + B\, e^{r/L}$
- Changing back to flux: $\Phi(r) = y(r) / r$
- General solution: $\Phi(r) = A\, e^{-r/L}/ r + B\, e^{r/L}/ r$
- Specific solution uses Boundary Conditions:

  (i) $\Phi(r) \rightarrow 0$, as $r \rightarrow \infty$ - thus $B = 0$

  (ii) *As* $r \rightarrow 0$, *no capture*, $J = - D\, d\Phi(r)/dr = S_o/4\pi r^2$

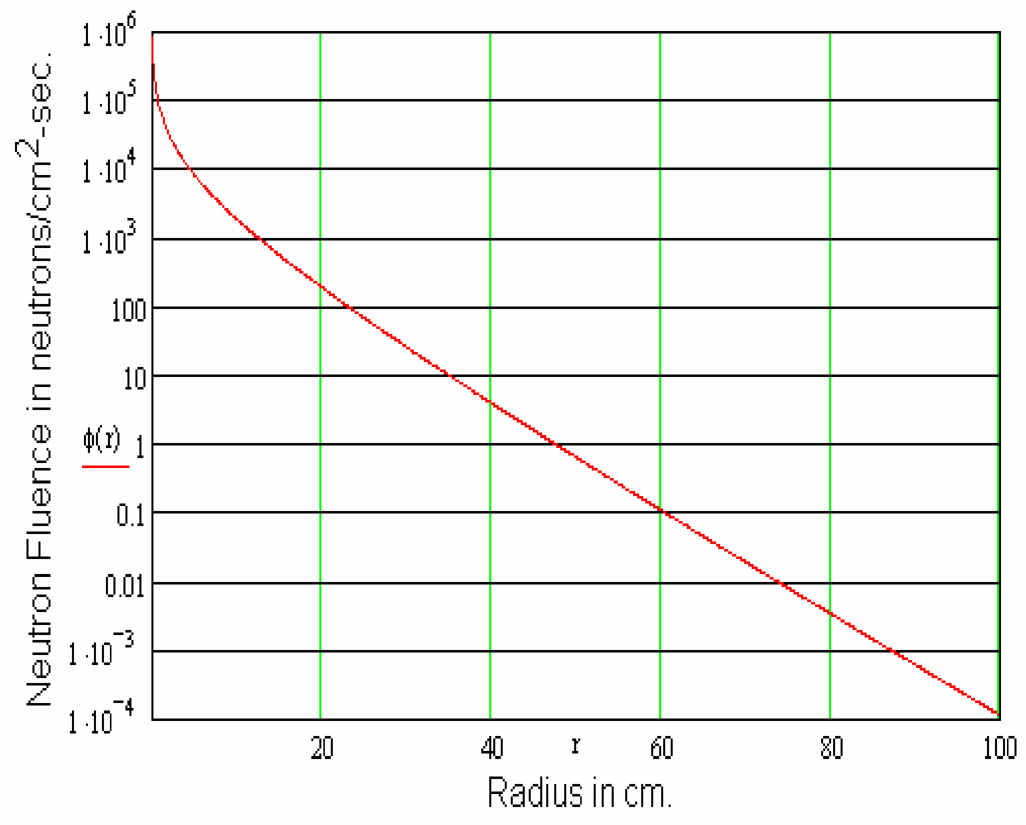
$$- D\, d\Phi(r)/dr = (DA / L\, r)\, e^{-r/L} + (DA / r^2)\, e^{-r/L} = S_o/4\pi r^2$$

- Canceling $r^2$ this is: $(DA\, r/ L)\, e^{-r/L} + (DA)\, e^{-r/L} = S_o/4\pi$
- Taking limit $r \rightarrow 0$, shows: $A = S_o/ 4\pi D$
- Thus: $\Phi(r) = S_o e^{-r/L} / 4\pi r D$

# *Diffusion from Point Neutron Source*

- Neutron source submerged in water emits $10^6$ thermal neutrons/sec
- $\Sigma_s = 3.45 cm^{-1}, \Sigma_c = 0.022 cm^{-1}$
- $D = 1/\Sigma_s(1-2/3) = 0.87 cm$
- $L = (D/\Sigma_c)^{1/2} = 6.287$

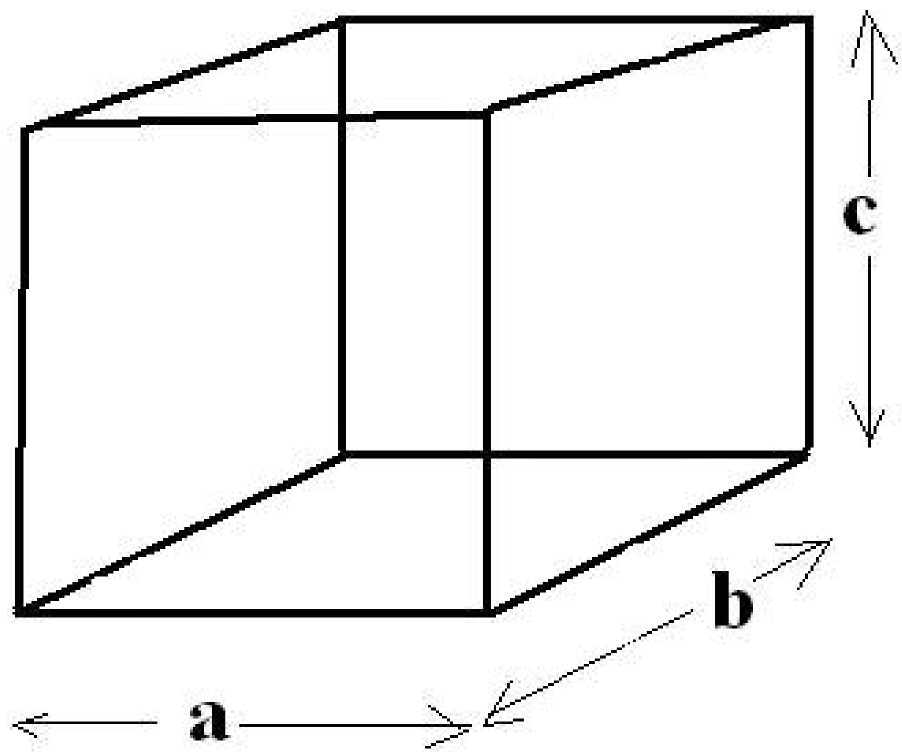
CAUTION: *we assumed thermal neutron source*.



# *Neutron Diffusion in Different Geometries*

- Laplacian operator for different geometries:
- Rectangular: $\partial^2\Phi/\partial x^2 + \partial^2\Phi/\partial y^2 + \partial^2\Phi/\partial z^2 - (\Sigma_c/D)\Phi = -S/D$
- Cylindrical: $\partial^2\Phi/\partial r^2 + (1/r)\,\partial\Phi/\partial r + \partial^2\Phi/\partial z^2 - (\Sigma_c/D)\Phi = -S/D$
- Spherical: $\partial^2\Phi/\partial r^2 + (2/r)\,\partial\Phi/\partial r - (\Sigma_c/D)\Phi = -S/D$

# *Cubical Reactor Geometry:*



# Separation of Variables Solution of 3-D Neutron Diffusion Equation

- Rectangular geometry: $a \cdot b \cdot c$
- Assume flux vanishes at edges: $(\pm a/2, \pm b/2, \pm c/2)$

$$\partial^2\Phi/\partial x^2 + \partial^2\Phi/\partial y^2 + \partial^2\Phi/\partial z^2 - (\Sigma_c/D)\Phi = -S/D$$

- Assume neutron source is: $S = \Sigma_c k\Phi$
- Assume: $\Phi(x,y,z) = F(x)G(y)H(z)$ *Equation becomes:*

$$G(y)H(z)\,\partial^2F/\partial x^2 + F(x)H(z)\,\partial^2G/\partial y^2 + F(x)G(y)\,\partial^2H/\partial z^2$$
$$= (\Sigma_c/D)(1-k)\,F(x)G(y)H(z)$$

- Dividing out: $F(x)G(y)H(z)$ from both sides yields:

$$(\partial^2F/\partial x^2)/F(x) + (\partial^2G/\partial y^2)/G(y) + (\partial^2H/\partial z^2)/H(z) = (\Sigma_c/D)(1-k)$$

# Separation of Variables Solution of 3-D Neutron Diffusion Equation

- Given boundary conditions: $F(\pm a/2) = 0, F(x) = \cos(x\pi/a)$
- Similarly: $G(y) = \cos(y\pi/b),\ H(z) = \cos(z\pi/c)$

$$(\partial^2 F/\partial x^2)/ F(x) = -(\pi/a)^2$$

$$(\partial^2 G/\partial y^2)/ G(y) = -(\pi/b)^2$$

$$(\partial^2 H/\partial z^2)/ H(z) = -(\pi/c)^2$$

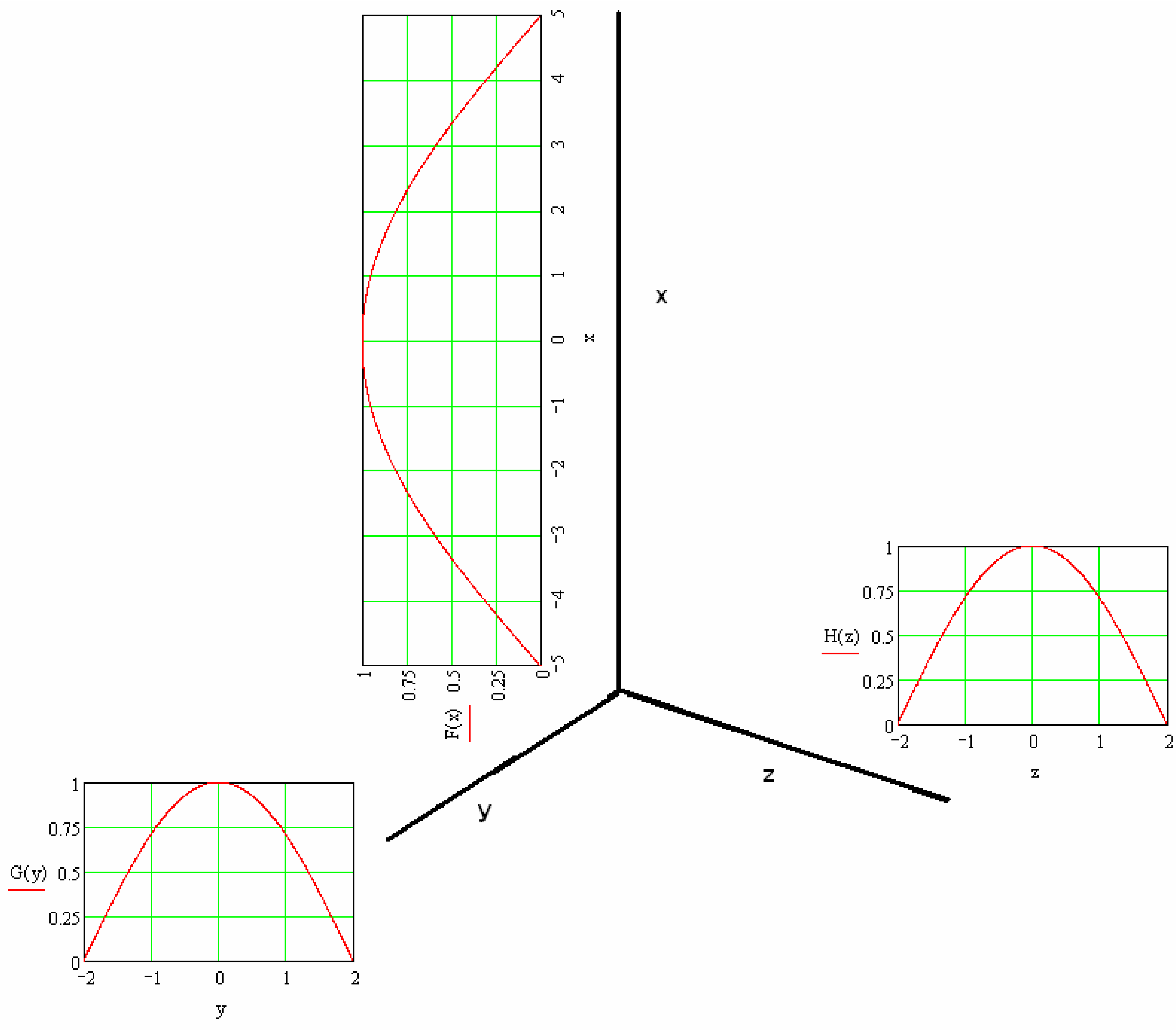
- Overall equation satisfies:

$$[(\pi/a)^2+(\pi/b)^2+(\pi/c)^2] = (\Sigma_c/D)(1-k)$$

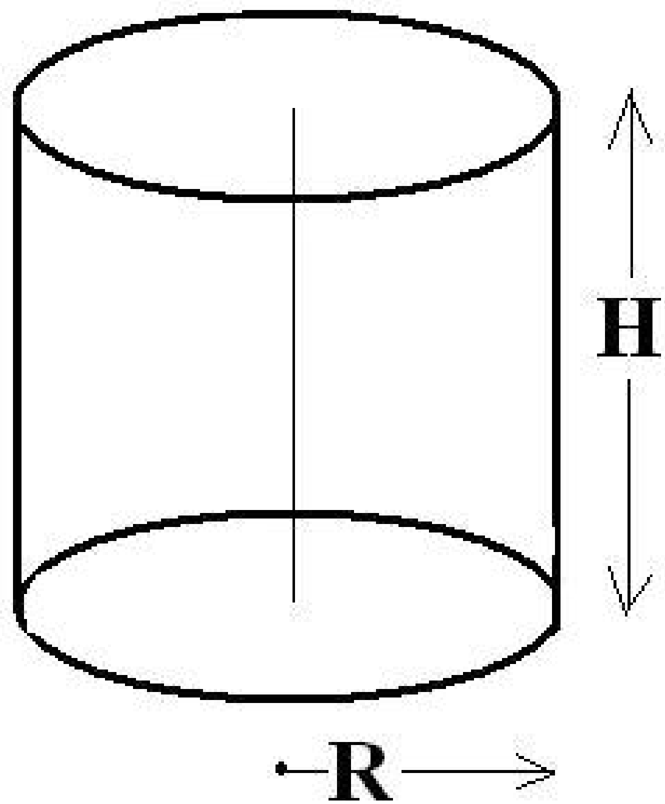
- Define *Geometrical Buckling*: $B^2 = [(\pi/a)^2+(\pi/b)^2+(\pi/c)^2]$
- $B^2$ is Eigenvalue of Helmholz-type equation:

$$\nabla^2\Phi + B^2\Phi = 0$$

# *Rectangular Flux Profile:* $\Phi(x,y,z) = F(x)G(y)H(z)$



# *Cylindrical Reactor Geometry:*



# *Separation of Variables Solution of 3-D Neutron Diffusion Equation*

- Separation of variables in cylindrical geometry proceeds in similar fashion
- Cylindrical dimensions: radius $= R$, Height $= H$
- Assume flux vanishes at: $(R, \pm H/2)$

$$\partial^2\Phi/\partial r^2+(1/r)\,\partial\Phi/\partial r+\partial^2\Phi/\partial z^2 - (\Sigma_c/D)\Phi = -S/D$$

- Assume: $\Phi(r,z) = F(r)G(z)$ *- equation becomes:*

$$[\partial^2F/\partial r^2+(1/r)\,\partial F/\partial r]\,G(z) + F(r)\,\partial^2G/\partial z^2$$
$$= -(\Sigma_c/D)(1-k)\,F(r)G(z)$$

- Dividing out $F(r)G(z)$ from both sides yields:

$$[\partial^2F/\partial r^2+(1/r)\,\partial F/\partial r]/F(r) + [\partial^2G/\partial z^2]/G(z)$$
$$= -(\Sigma_c/D)(1-k)$$

# *Separation of Variables Solution of 3-D Neutron Diffusion Equation*

- Axial portion is similar to that of cubical geometry:

$$(\partial^2 G/\partial z^2)/\, G(z) = -\, (\pi/H)^2 \;\rightarrow\; G(z) = \cos(z\pi/H)$$

- Radial portion involves *Bessel Function of first kind*:

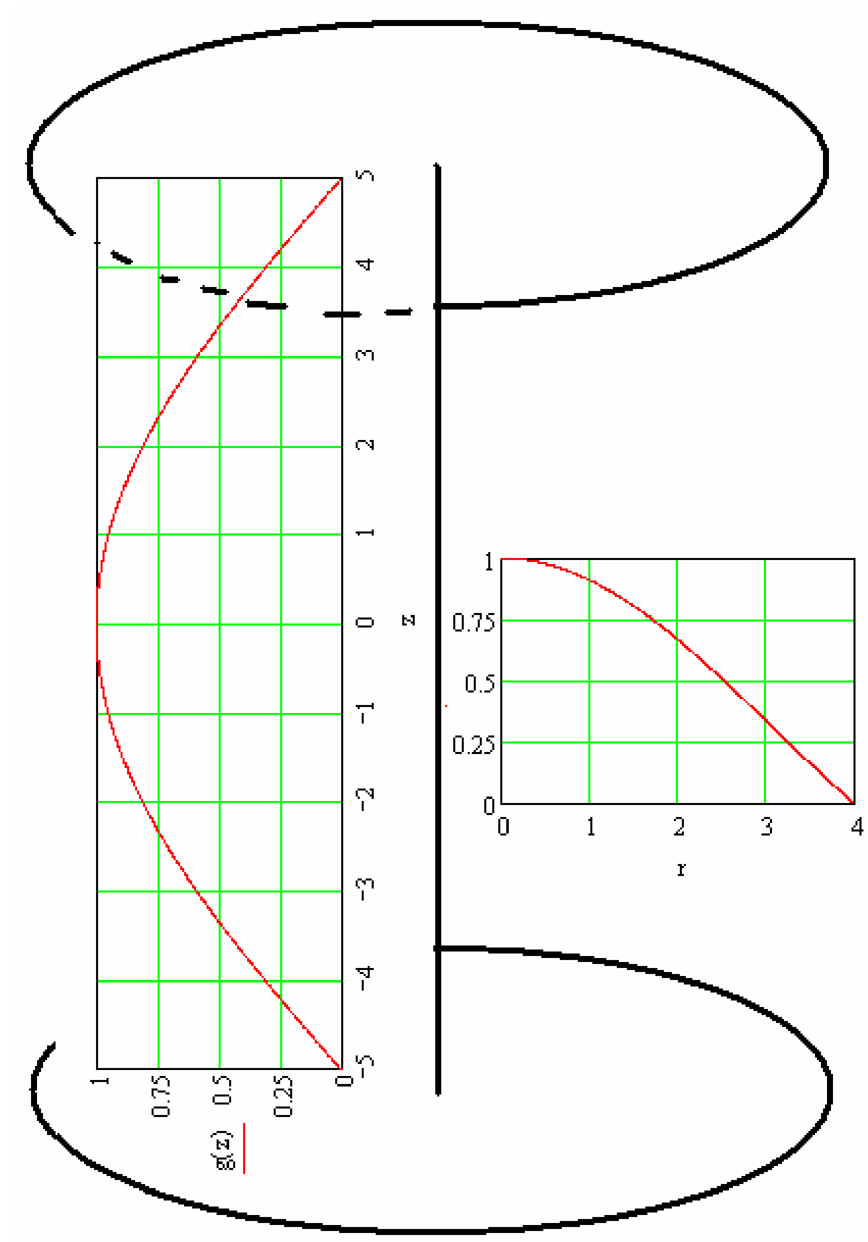
$$[\partial^2 F/\, \partial r^2 + (1/r)\, \partial F/\, \partial r]/\, F(r) = -\, (2.405/R)^2$$

$$F(r) = J_o(2.405\, r\, /\, R)$$

- Overall Geometrical Buckling for a cylinder is expressed:

$$B^2 = [(2.405/R)^2 + (\pi/H)^2\, ]$$

# Cylindrical Flux Profile: $\Phi(r,z) = F(r)G(z)$



# *Geometrical Buckling for Other Geometries*

- Geometrical Buckling factor captures surface to volume effects of different geometries
- Buckling factors are for *bare*, *un-reflected* systems:

| Geometry: | Dimensions: | Buckling: | Flux Shape: |
|---|---|---|---|
| Rectangular Block | $a \times b \times c$ | $B^2 = \left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2$ | $\phi(x,y,z) = A_0 \cos\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi y}{b}\right)\cos\left(\frac{\pi z}{c}\right)$ |
| Sphere | $Radius : R$ | $B^2 = \left(\frac{\pi}{R}\right)^2$ | $\phi(r) = \frac{A_0}{r}\sin\left(\frac{\pi r}{R}\right)$ |
| Cylinder | $Radius : R$ $Height : H$ | $B^2 = \left(\frac{2.405}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2$ | $\phi(r,z) = A_0 J_0\left(\frac{2.405 r}{R}\right)\cos\left(\frac{\pi z}{H}\right)$ |

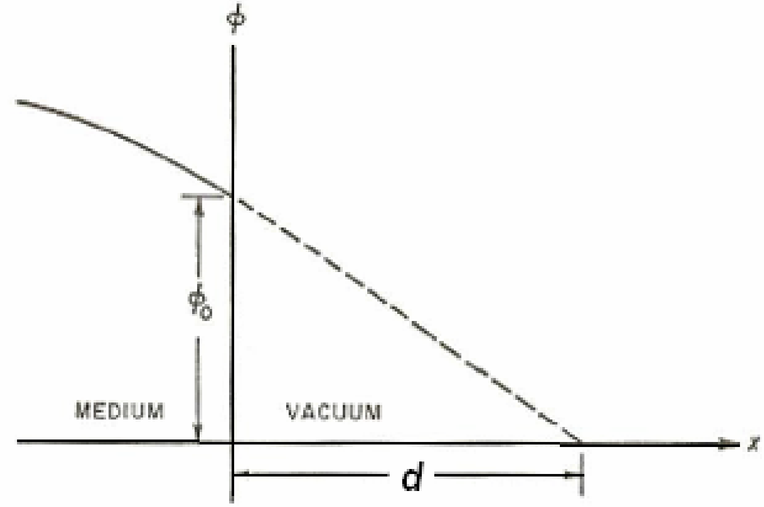
*Taken from: J. Lamarsh, "Nuclear Reactor Analysis, p.298*

# *Vacuum Boundary Correction*

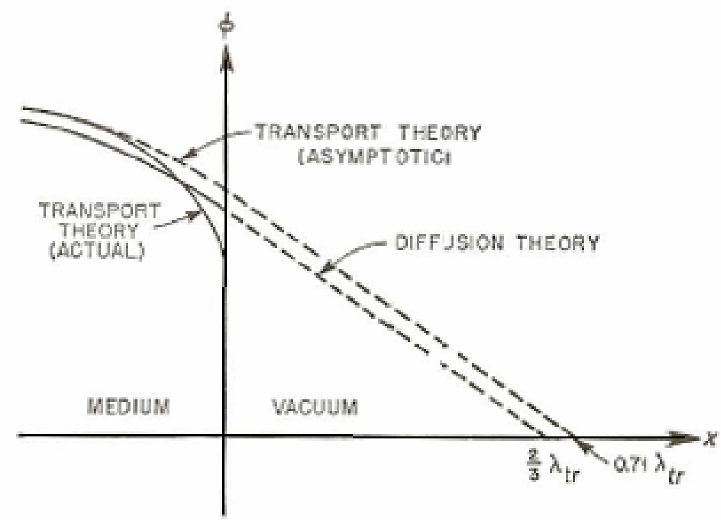
# *Vacuum Boundary Condition Approximation*

- Simple diffusion calculations have assumed $\Phi$ vanishes at boundary
- Obviously neutrons will stream out of core region at boundary unless *reflected back*
- Flux $\Phi$ would vanish at distance *"d"* given by: $d\Phi/dx = - \Phi_o / d$
- Solving for current at boundary via diffusion approximation yields: $d \sim 2l$
- Since: $D = (1/3)\lambda_{tr}$ ($\lambda_{tr}$ is mean free transport length) - thus: $d \sim (2/3)\lambda_{tr}$
- Detailed numerical analysis via transport methods indicate:

  $d = 0.71\ \lambda_{tr}$




*Extrapolation of Neutron Flux at Multiplying Medium Boundary*

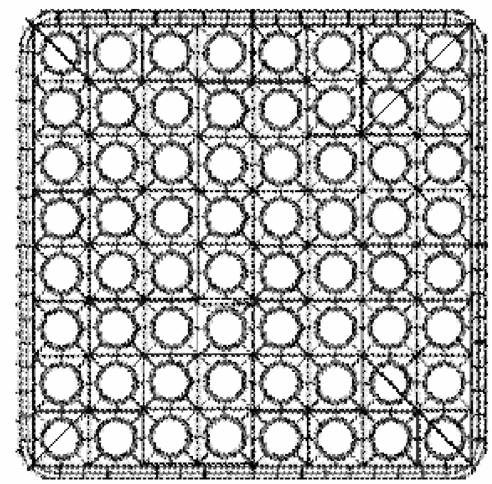


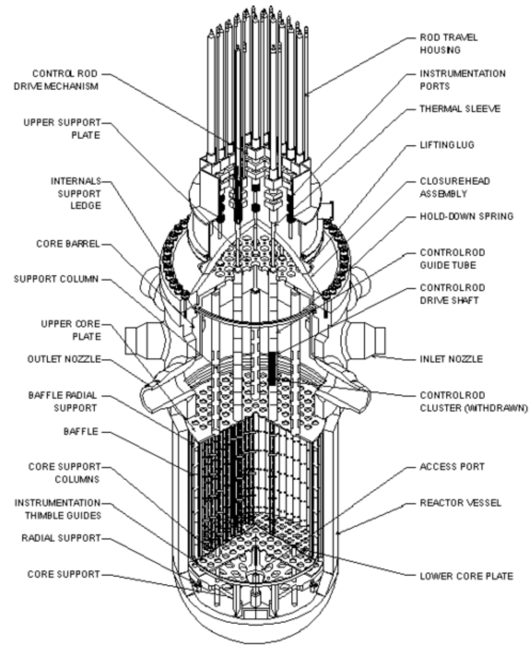

*Transport Theory vs. Diffusion Theory Extrapolation at Boundary of Multiplying Medium*

# *Corrections Needed for Deviations from Transport Equation Simplification*

- We "casually" employed some assumptions *not consistent* with transport equation simplifications
- "No discontinuities"
- Diffusion constant does not vary spatially
- *Multiplying media is highly discontinuous*
- Small Gradient terms: $d\Phi/dr$

  Maybe not so bad – but depends on previous item
- Assumption of bare, non-reflecting media implies high neutron leakage
- Power reactors designed to reduce leakage via neutron reflector





# *Multi-Group Diffusion: Need for Numerical Models*

- One Group Diffusion Model reasonably predicts thermal flux in *simple uniform geometries*
- Analyzing effects of flux depression near fuel pellets or control rods (very strong absorbers) necessitates considering multiple neutron groups
- Simplest form is 2-Group Diffusion model:

$$0 = S_f - \phi_f \Sigma_{a-f} + D_f \nabla^2 \phi_f \qquad 0 = S_{th} - \phi_{th} \Sigma_{a-th} + D_{th} \nabla^2 \phi_{th}$$

- Fast neutron source is from fast and thermal fission
- Thermal neutron source is thermalized fast neutrons
- *We will use this model in future to discuss critical conditions*

# *Multi-Group Diffusion: Need for Numerical Models*

- Consideration of many neutron groups improves accuracy but adds numerical computation complexity

- *Additional sources*: scattering in from other energy groups

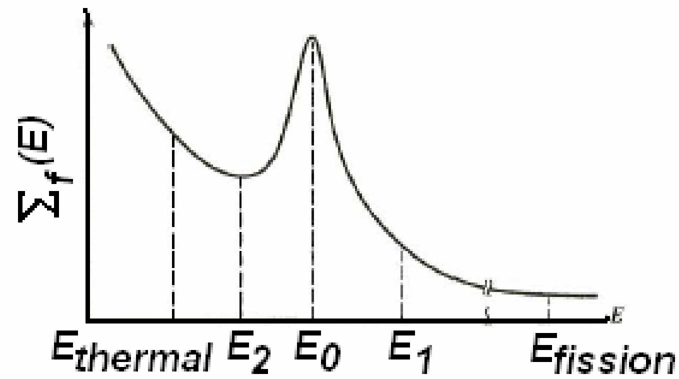
- *Additional sinks*: scattering out to other energy groups

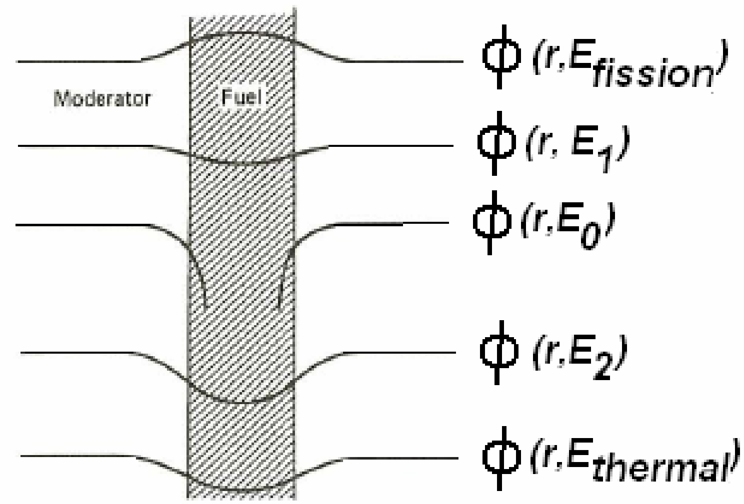
- Multi-group diffusion equations are solved via numerical matrix solvers

# *Example Application of Multi-Group Diffusion*

- Suppose we want to understand temperature distribution within fuel pellet
- Thermal neutrons strongly absorbed as they move from moderator into fuel pellet
- This causes *flux depression*
- Fission neutrons leak out of fuel quickly
- Fast flux is peaked in center
- Heat generation within pellet:

$$q(r) \sim \sum \Phi(r,E_i)\Sigma_f(E_i)E_{fission}$$

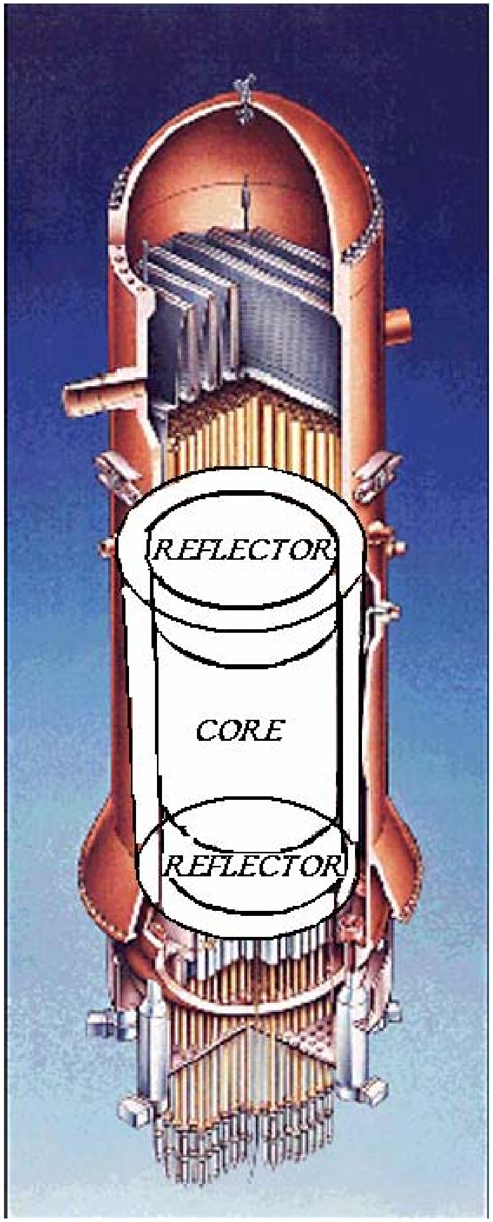


*Multigroup Flux behavior in a fuel pellet*

*Modeling of Reflectors*

# *Reflector Region is Water Outside Reactor Core*



# *Modeling Reflector Involves System of Equations*

- Two region system of diffusion equations:

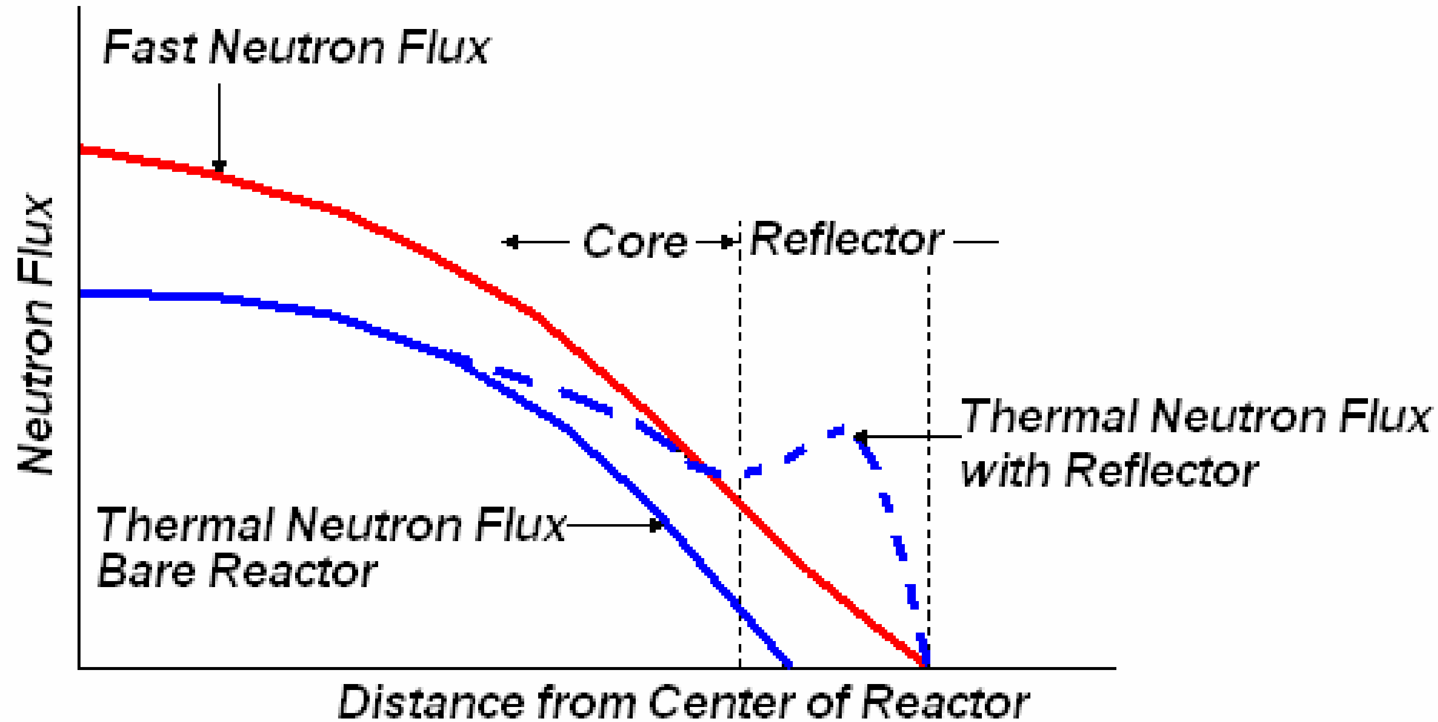
$$k\Sigma_{ac}\phi_c = \Sigma_{ac}\phi_c - D_c\nabla^2\phi_c$$

$$0 = \Sigma_{ar}\phi_r - D_r\nabla^2\phi_r$$

- - no neutron source within reflector region
- Subscript "$c$" refers to core region, "$r$" refers to reflector region
- Boundary conditions at edge of core must match: $\Phi_c(R_c) = \Phi_r(R_c)$
- Flux gradient must not *be* discontinuous at edge: $d\Phi_c/dr(R_c) = d\Phi_r/dr(R_c)$
- *Problem:* We should consider fast neutrons leaking from core but thermalizing in reflector region and bouncing back into core region

# *Modeling Reflector Involves System of Equations*

- At this point we must jump to *numerical solution!*
- Escaping fast neutron flux readily thermalizes in water region
- Increased thermal neutrons in reflector raises flux at periphery of reactor core



# *Limitations of Diffusion Theory*

- Stacey notes in *Nuclear Reactor Physics* (p. 49):
- "Diffusion theory is a strictly valid mathematical description of neutron flux….*when assumptions used in derivation are satisfied*."
- Absorption is less likely in moderator region, hence flux shape in moderator region is *reasonably accurate*
- Flux within fuel pellets is impacted by very strong neutron absorption, hence *flux shape in fuel pellets less accurate*
- Diffusion theory is widely used in reactor analysis
- *SECRET:* "use transport theory to make diffusion theory work in specific areas where it would be expected to fail"
- "Numerous small elements in reactor are replaced by homogenized mixture with effective averaged cross sections and diffusion coefficients"

# *Summary*

- Neutron diffusion theory works well *outside of fuel pellets*
- Neutron diffusion originates from Boltzmann's equation
- Neutron diffusion models: neutron sources, sinks, leakage at periphery
- General approach is to develop *energy group dependent constants* for: $D$, $\Sigma_t$ , $\Sigma_a$
- Diffusion theory is pretty good explaining general reactor neutron flux profiles
- Reactor physicists know how to correct *known weaknesses* of diffusion theory via *adjustments*