NUCL 510
Nuclear Reactor Theory

Fall 2011
Lecture Note 5

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Diffusion Equation

- Continuous energy diffusion equation

$$-\nabla \cdot D(\vec{r},E)\nabla\phi(\vec{r},E)+\Sigma_t(\vec{r},E)\phi(\vec{r},E)$$
$$=\chi(E)\int_{E'} dE'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E')+\int_{E'} dE'\Sigma_s(\vec{r},E'\rightarrow E)\phi(\vec{r},E')+S(\vec{r},E)$$

- Interface conditions

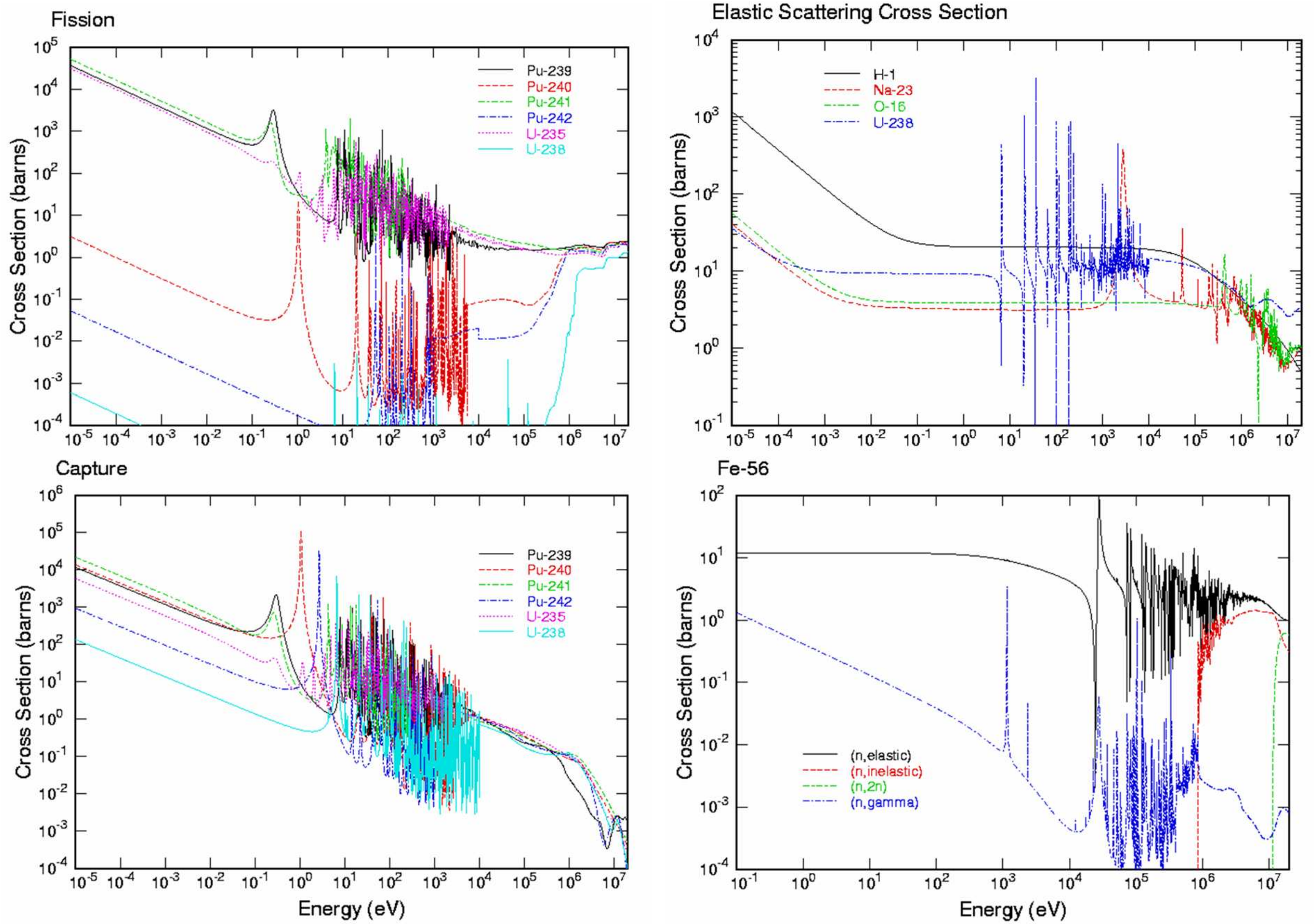
$$\phi(\vec{r}_i^{\,-},E)=\phi(\vec{r}_i^{\,+},E) \quad \text{(continuity of flux)}$$
$$\vec{n}\cdot D(\vec{r}_i^{\,-},E)\nabla\phi(\vec{r}_i^{\,-},E)=\vec{n}\cdot D(\vec{r}_i^{\,+},E)\nabla\phi(\vec{r}_i^{\,+},E) \quad \text{(continuity of normal current)}$$

- Vacuum boundary condition

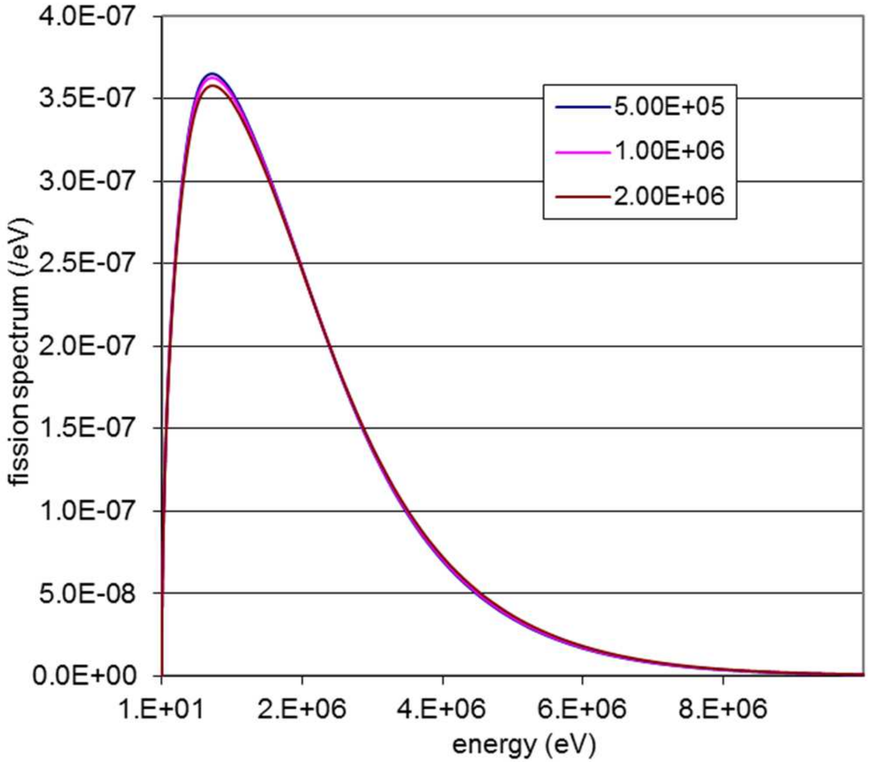
$$\phi(\vec{r}_v+0.711\lambda_{tr}\vec{n},E)=0$$

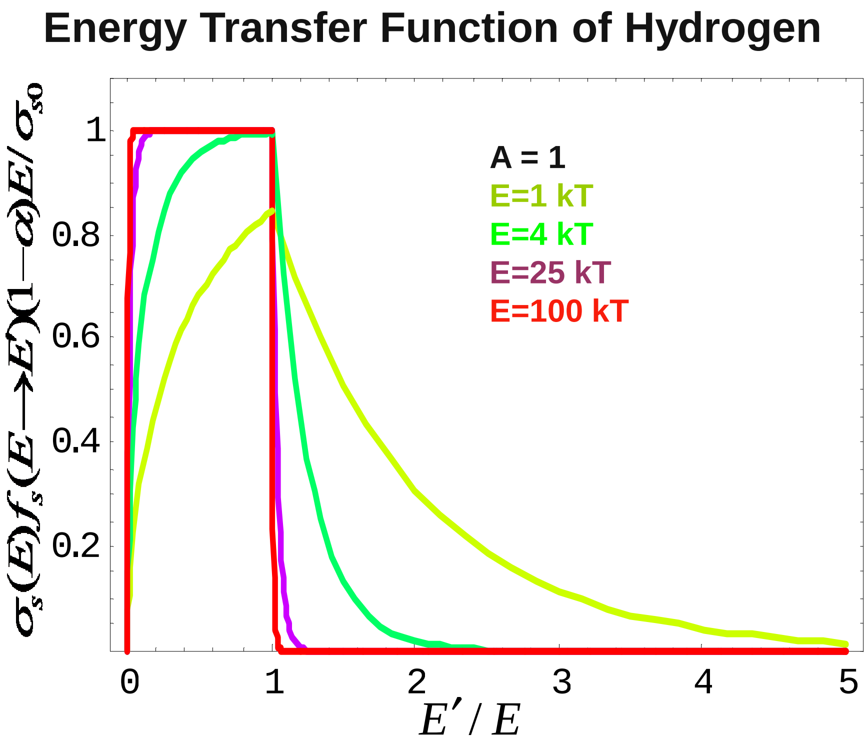
- Diffusion theory approximation of current is inaccurate or invalid when free diffusion of neutrons is inhibited
  - In strong absorption regions (e.g., control blades or rods)
  - At boundaries between materials with very different cross sections
  - At a concentrated neutron source (point or plane source)
  - Near a vacuum boundary

Cross Sections



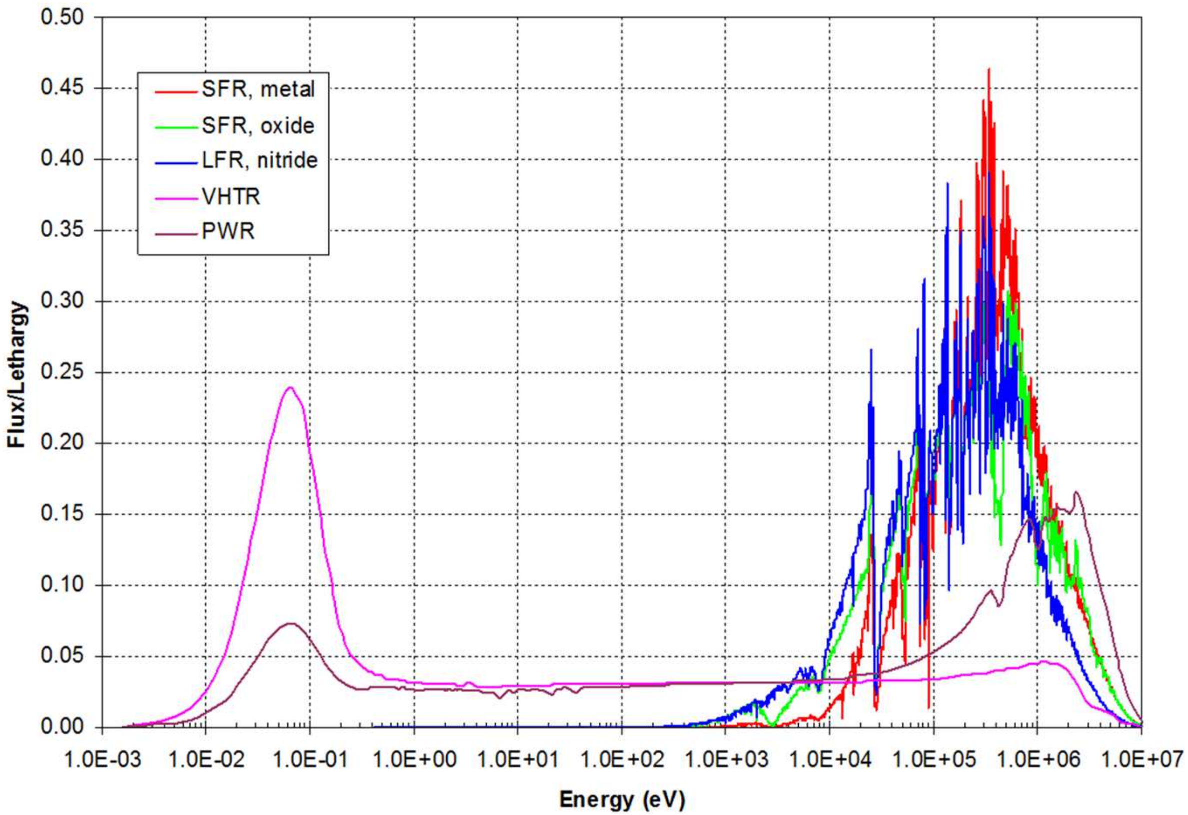
Energy Distributions of Fission and Scattered Neutrons





- Fission neutrons with average energy of ~2 MeV lose energy by scattering with materials in the reactor

Typical Neutron Spectra



- Lethargy

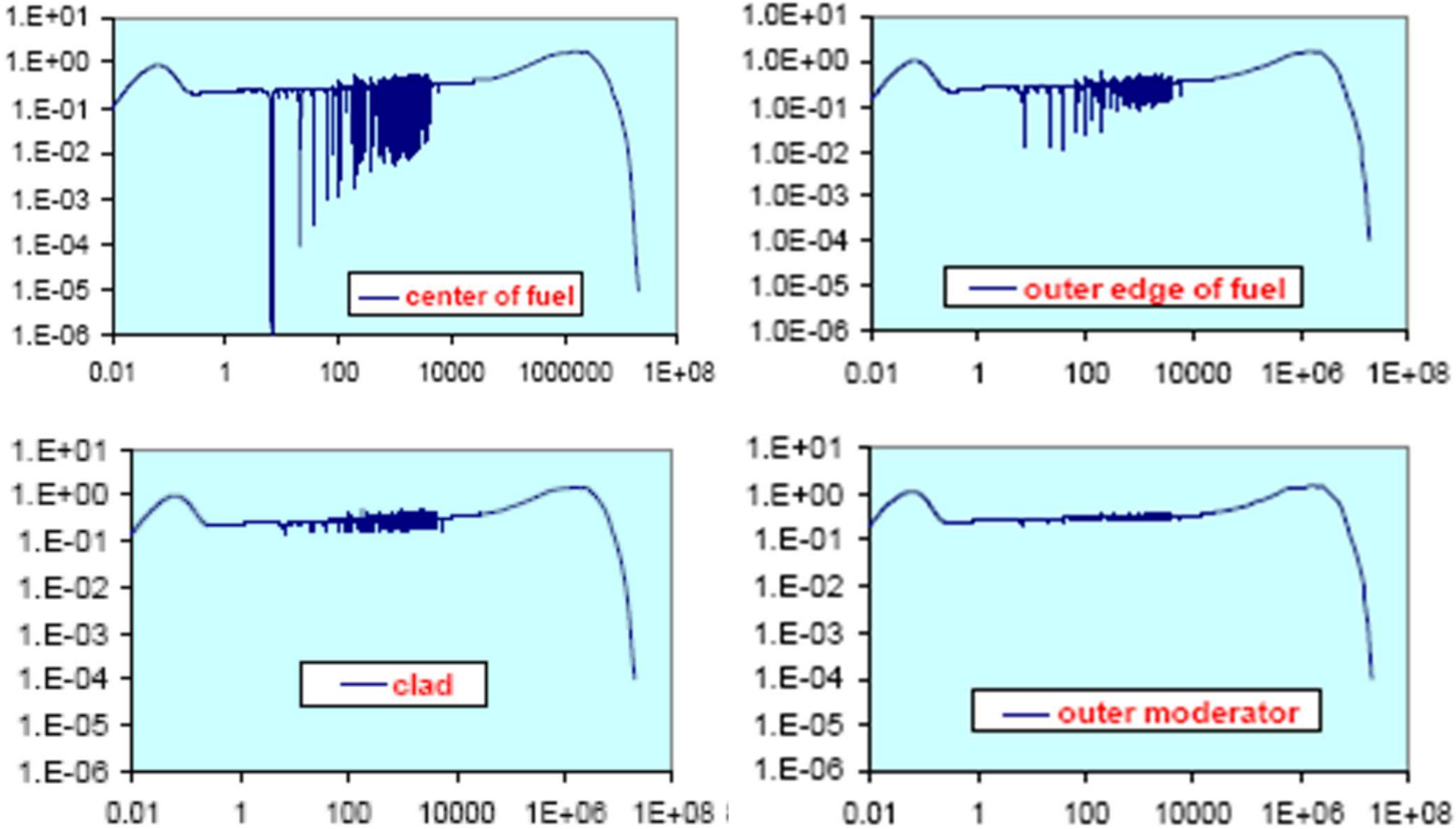
  $$u = \ln \frac{E_0}{E}$$

  E_0 = arbitrary initial energy (e.g., 10 MeV)

- Lethargy increases as energy decreases

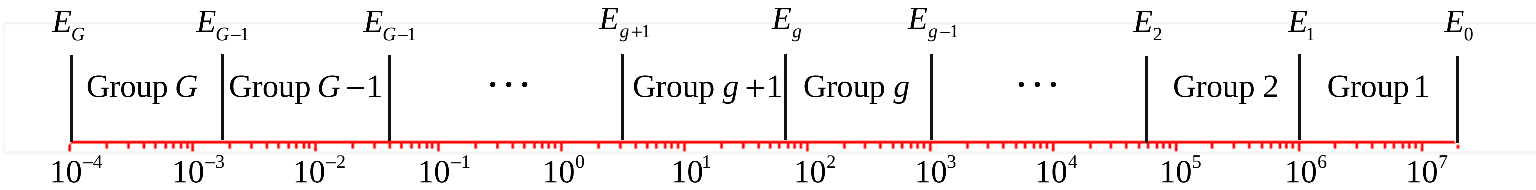
- In thermal reactors, neutron moderation is enhanced by the use of low atomic mass materials
- In fast reactors, neutron moderation is minimized by the use of high atomic mass materials, and thus neutrons are either absorbed or leak out from the core before they reach thermal energies

LWR Pin Cell Spectrum (CENTRM)



Multi-group Approach

- Divide the energy range into several intervals
  - Each interval is called a group



- Define the <u>unknown</u> group fluxes by the integrals of the flux over individual intervals

$$\phi_g(\vec{r}) = \int_{E_g}^{E_{g-1}} \phi(\vec{r}, E)\,dE$$

- Group average cross sections (or group constants) are defined in such way that the reaction rates in each interval are preserved

$$\sigma_{xg}^{i}(\vec{r}) = \frac{1}{\phi_g(\vec{r})}\int_{E_g}^{E_{g-1}} \sigma_x^i(\vec{r}, E)\phi(\vec{r}, E)\,dE = \frac{\int_{E_g}^{E_{g-1}} \sigma_x^i(\vec{r}, E)\phi(\vec{r}, E)\,dE}{\int_{E_g}^{E_{g-1}} \phi(\vec{r}, E)\,dE}$$

  - The group constants are typically determined using the neutron spectra obtained by solving local problems with approximate boundary conditions

Derivation of Multi-group Diffusion Equation (1)

- Integration of continuous energy diffusion equation

$$-\int_{E_g}^{E_{g-1}} dE\nabla\cdot D(\vec{r},E)\nabla\phi(\vec{r},E)+\int_{E_g}^{E_{g-1}} dE\Sigma_t(\vec{r},E)\phi(\vec{r},E)=\int_{E_g}^{E_{g-1}} dES(\vec{r},E)$$
$$+\int_{E_g}^{E_{g-1}} dE\chi(E)\int_{E'} dE'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E')+\int_{E_g}^{E_{g-1}} dE\int_{E'} dE'\Sigma_s(\vec{r},E'\rightarrow E)\phi(\vec{r},E')$$

- Total reaction term

$$\int_{E_g}^{E_{g-1}} dE\Sigma_t(\vec{r},E)\phi(\vec{r},E)=\Sigma_{tg}(\vec{r})\int_{E_g}^{E_{g-1}} dE\phi(\vec{r},E)=\Sigma_{tg}(\vec{r})\phi_g(\vec{r})$$

$$\Sigma_{tg}(\vec{r})=\sum_i N_i(\vec{r})\sigma_{tg}^i(\vec{r})$$

$$\sigma_{tg}^i(\vec{r})=\frac{1}{\phi_g(\vec{r})}\int_{E_g}^{E_{g-1}}\sigma_t^i(E)\phi(\vec{r},E)dE=\frac{\int_{E_g}^{E_{g-1}}\sigma_t^i(E)\phi(\vec{r},E)dE}{\int_{E_g}^{E_{g-1}}\phi(\vec{r},E)dE}$$

$$\sigma_{xg}^i(\vec{r})\equiv\frac{1}{\phi_g(\vec{r})}\int_{E_g}^{E_{g-1}}\sigma_{xg}^i(E)\phi(\vec{r},E)dE \quad (x=c,f,a,s)$$

- Independent source term $\int_{E_g}^{E_{g-1}} dES(\vec{r},E)=S_g(\vec{r})$

Derivation of Multi-group Diffusion Equation (2)

- Fission source term

$$\int_{E_g}^{E_{g-1}} dE\,\chi(E)\int_{E'} dE'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E') = \chi_g S_f(\vec{r}) \quad (S_f = \text{total fission source at } \vec{r})$$

$$S_f(\vec{r}) = \int_{E'} dE'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E') = \sum_{g'=1}^{G}\int_{E_g}^{E_{g-1}} dE'\nu\Sigma_f(\vec{r},E')\phi(\vec{r},E') = \sum_{g'=1}^{G}\nu\Sigma_{fg}(\vec{r})\phi_g(\vec{r})$$

$$\chi_g = \int_{E_g}^{E_{g-1}} dE\,\chi(E)$$

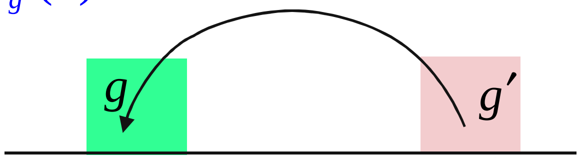
$$\nu\sigma_{fg}^i(\vec{r}) = \frac{1}{\phi_g(\vec{r})}\int_{E_g}^{E_{g-1}} \nu(E)\sigma_f^i(E)\phi(\vec{r},E)dE$$

- Scattering source term

$$\int_{E_g}^{E_{g-1}} dE\int_{E'} dE'\Sigma_s(\vec{r},E'\to E)\phi(\vec{r},E')dE = \int_{E_g}^{E_{g-1}} dE\sum_{g'=1}^{G}\int_{E_{g'}}^{E_{g'-1}} dE'\Sigma_s(\vec{r},E'\to E)\phi(\vec{r},E')$$

$$= \sum_{g'=1}^{G}\int_{E_g}^{E_{g-1}} dE\int_{E_{g'}}^{E_{g'-1}} dE'\Sigma_s(\vec{r},E'\to E)\phi(\vec{r},E') = \sum_{g'=1}^{G}\Sigma_{sg'g}(\vec{r})\phi_{g'}(\vec{r})$$

$$\sigma_{sg'g}^i(\vec{r}) = \frac{1}{\phi_{g'}(\vec{r})}\int_{E_g}^{E_{g-1}} dE\int_{E_{g'}}^{E_{g'-1}} dE'\sigma_s^i(E'\to E)\phi(\vec{r},E')$$



transfer from g to g'

Derivation of Multi-group Diffusion Equation (3)

- Diffusion term

$$\int_{E_g}^{E_{g-1}} dE \nabla \cdot D(\vec{r}, E)\nabla\phi(\vec{r}, E) = \nabla \cdot D_g(\vec{r}) \int_{E_g}^{E_{g-1}} dE \nabla\phi(\vec{r}, E) = \nabla \cdot D_g(\vec{r})\nabla\phi_g(\vec{r})$$

$$\mathbf{D}_g(\vec{r})\nabla\phi_g(\vec{r}) = \int_{E_g}^{E_{g-1}} dE D(\vec{r}, E)\nabla\phi(\vec{r}, E)$$

  - In general, the group diffusion coefficients $\mathbf{D}_g$ should be a tensor (3×3 symmetric matrix, Eddington tensor)

$$\mathbf{D}_g(\vec{r}) = \begin{bmatrix} D_g^{xx} & D_g^{xy} & D_g^{xz} \\ D_g^{xy} & D_g^{yy} & D_g^{yz} \\ D_g^{xz} & D_g^{xy} & D_g^{zz} \end{bmatrix}$$

  - The diffusion tensor is approximated by a diagonal matrix, which yields directional diffusion coefficients

$$D_g^{\alpha}(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} dE D(\vec{r}, E)\frac{\partial}{\partial\alpha}\phi(\vec{r}, E)}{\frac{\partial}{\partial\alpha}\phi_g}, \quad \alpha = x, y, z$$

  - Directional diffusion coefficients are generally similar, and thus they are approximated by direction-independent one

Multi-group Diffusion Equation

- Multi-group diffusion equation

$$-\nabla \cdot D_g(\vec{r})\nabla\phi_g(\vec{r}) + \Sigma_{tg}(\vec{r})\phi_g(\vec{r}) = \chi_g \sum_{g'=1}^{G} \nu\Sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r}) + \sum_{g'=1}^{G} \Sigma_{sg'g}(\vec{r})\phi_{g'}(\vec{r}) + S_g(\vec{r}),$$

$$g = 1, 2, \cdots, G$$

- Cancellation of within-group scattering
  - The within-group scattering (or self scattering) term appears on both sides

$$\Sigma_{tg} = \Sigma_{ag} + \Sigma_{sg} = \Sigma_{ag} + \sum_{g'=1}^{G} \Sigma_{sgg'}$$

- Removal cross section

$$\Sigma_{rg} = \Sigma_{tg} - \Sigma_{sgg} = \Sigma_{a,g} + \sum_{\substack{g'=1 \\ g' \neq g}}^{G} \Sigma_{sg'g}$$

- Multi-group diffusion equation in terms of removal cross section

$$-\nabla \cdot D_g(\vec{r})\nabla\phi_g(\vec{r}) + \Sigma_{rg}(\vec{r})\phi_g(\vec{r}) = \chi_g \sum_{g'=1}^{G} \nu\Sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r}) + \sum_{\substack{g'=1 \\ g' \neq g}}^{G} \Sigma_{sg'g}(\vec{r})\phi_{g'}(\vec{r}) + S_g(\vec{r}),$$

$$g = 1, 2, \cdots, G$$

Matrix Representation (1)

- Loss terms

$$-\nabla\cdot D_g(\vec{r})\nabla\phi_g(\vec{r})+\Sigma_{rg}(\vec{r})\phi_g(\vec{r}),\quad g=1,2,\cdots,G$$

$$\Rightarrow\begin{bmatrix}-\nabla\cdot D_1(\vec{r})\nabla+\Sigma_{r1}(\vec{r}) & 0 & \cdots & 0\\ 0 & -\nabla\cdot D_2(\vec{r})\nabla+\Sigma_{r2}(\vec{r}) & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & -\nabla\cdot D_G(\vec{r})\nabla+\Sigma_{rG}(\vec{r})\end{bmatrix}\begin{bmatrix}\phi_1(\vec{r})\\ \phi_2(\vec{r})\\ \vdots\\ \phi_G(\vec{r})\end{bmatrix}$$

$$=\mathbf{L}\boldsymbol{\varphi}$$

- Scattering source (without self-scattering source)

$$\sum_{g'\neq g}\Sigma_{sg'g}(\vec{r})\phi_{g'}(\vec{r}),\quad g=1,2,\cdots,G$$

$$\Rightarrow\begin{bmatrix}0 & \Sigma_{s21}(\vec{r}) & \cdots & \Sigma_{sG1}(\vec{r})\\ \Sigma_{s12}(\vec{r}) & 0 & \cdots & \Sigma_{sG2}(\vec{r})\\ \vdots & \vdots & \ddots & \vdots\\ \Sigma_{s1G}(\vec{r}) & \Sigma_{s2G}(\vec{r}) & \ldots & 0\end{bmatrix}\begin{bmatrix}\phi_1(\vec{r})\\ \phi_2(\vec{r})\\ \vdots\\ \phi_G(\vec{r})\end{bmatrix}\qquad \mathbf{S}=\begin{bmatrix}\Sigma_{s11}(\vec{r}) & \Sigma_{s21}(\vec{r}) & \cdots & \Sigma_{sG1}(\vec{r})\\ \Sigma_{s12}(\vec{r}) & \Sigma_{s22}(\vec{r}) & \cdots & \Sigma_{sG2}(\vec{r})\\ \vdots & \vdots & \ddots & \vdots\\ \Sigma_{s1G}(\vec{r}) & \Sigma_{s2G}(\vec{r}) & \ldots & \Sigma_{sGG}(\vec{r})\end{bmatrix}$$

$$=\tilde{\mathbf{S}}\boldsymbol{\varphi}$$

Matrix Representation (2)

- Fission source term

$$\chi_g \sum_{g'=1}^{G} \nu\Sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r}), \quad g = 1, 2, \cdots, G$$

$$S_f(\vec{r}) = \sum_{g'=1}^{G} \nu\Sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r}) = \mathbf{f}^T \boldsymbol{\varphi}$$

$$\Rightarrow \begin{bmatrix} \chi_1 \\ \chi_2 \\ \vdots \\ \chi_G \end{bmatrix} S_f(\vec{r}) = \boldsymbol{\chi} S_f(\vec{r}) \qquad \mathbf{f}(\vec{r}) = \begin{bmatrix} \nu\Sigma_{f1}(\vec{r}) \\ \nu\Sigma_{f2}(\vec{r}) \\ \vdots \\ \nu\Sigma_{fG}(\vec{r}) \end{bmatrix}$$

$$\boldsymbol{\chi} S_f = \boldsymbol{\chi}\mathbf{f}^T \boldsymbol{\varphi} = \mathbf{F}\boldsymbol{\varphi}$$

$$\mathbf{F} = \chi \mathbf{f}^T = \begin{bmatrix} \chi_1 \\ \chi_2 \\ \vdots \\ \chi_G \end{bmatrix} \begin{bmatrix} \nu\Sigma_{f1} & \nu\Sigma_{f2} & \cdots & \nu\Sigma_{fG} \end{bmatrix} = \begin{bmatrix} \chi_1\nu\Sigma_{f1} & \chi_1\nu\Sigma_{f2} & \cdots & \chi_1\nu\Sigma_{fG} \\ \chi_2\nu\Sigma_{f1} & \chi_2\nu\Sigma_{f2} & \cdots & \chi_2\nu\Sigma_{fG} \\ \vdots & \vdots & \ddots & \vdots \\ \chi_G\nu\Sigma_{f1} & \chi_G\nu\Sigma_{f2} & \cdots & \chi_G\nu\Sigma_{fG} \end{bmatrix}$$

- Matrix form of multi-group diffusion equation

$$\mathbf{L}\boldsymbol{\varphi} = \mathbf{F}\boldsymbol{\varphi} + \tilde{\mathbf{S}}\boldsymbol{\varphi} + \mathbf{s}$$

$$\mathbf{M}\boldsymbol{\varphi} = \mathbf{F}\boldsymbol{\varphi} + \mathbf{s}, \quad \mathbf{M} = \mathbf{L} - \tilde{\mathbf{S}}$$

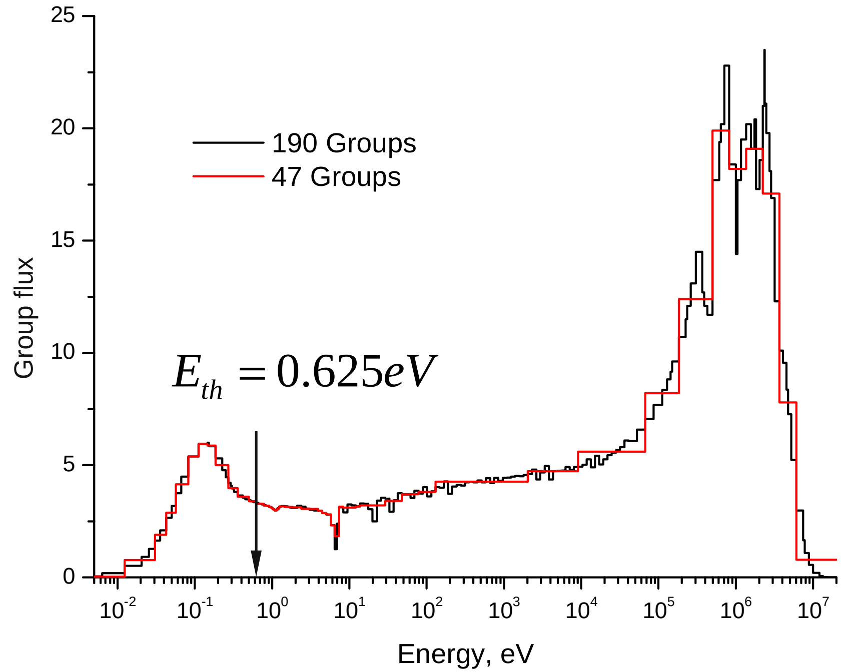
$$\mathbf{s}(\vec{r}) = \begin{bmatrix} S_1(\vec{r}) \\ S_2(\vec{r}) \\ \vdots \\ S_G(\vec{r}) \end{bmatrix}$$

Multi-group Solution Approach

- Generate multi-group cross sections <u>in advance</u>
  - It is assumed that within-group spectrum is not so sensitive to specific conditions
  - Spectrum is determined by solving a localized problem with a simplified boundary condition (e.g., 2-D assembly calculation with reflective BC)
  - Valid if the effects of neighboring compositions are small
  - More groups are required if the neighbor effects become larger

$$G_{FBR} \gg G_{LWR}$$

- Solve for group fluxes
  - Relative ratio among group fluxes changes largely due to the interaction effects with neighboring compositions



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Two-Group Diffusion Equation

- Group structure for LWR analysis
  - Group 1: E $\geq$ 0.625 eV $\rightarrow$ fast group
  - Group 2: E < 0.625 eV $\rightarrow$ thermal group
- Fission source
  - Total fission source

$$S_f(\vec{r}) = \nu\Sigma_{f1}(\vec{r})\phi_1(\vec{r}) + \nu\Sigma_{f2}(\vec{r})\phi_2(\vec{r})$$

  - In general, χ_1=1.0 and χ_2=0.0 $\rightarrow$ fission source in thermal group = 0
- Scattering source
  - Up-scattering is generally negligible; no scattering source into group 1

$$\Sigma_{21}(\vec{r}) = 0$$

- Two-group diffusion equation

$$-\nabla \cdot D_1(\vec{r})\nabla\phi_1(\vec{r}) + \Sigma_{r1}(\vec{r})\phi_1(\vec{r}) = \nu\Sigma_{f1}(\vec{r})\phi_1(\vec{r}) + \nu\Sigma_{f2}(\vec{r})\phi_2(\vec{r}) + s_1(\vec{r})$$
$$-\nabla \cdot D_2(\vec{r})\nabla\phi_2(\vec{r}) + \Sigma_{r2}(\vec{r})\phi_2(\vec{r}) = \Sigma_{s12}(\vec{r})\phi_1(\vec{r}) + s_2(\vec{r})$$

$$\Sigma_{r1} = \Sigma_{a1} + \Sigma_{s12}, \quad \Sigma_{r2} = \Sigma_{a2}$$

Multi-group Constants for Transport Equation

- Multi-group cross sections

$$\sigma^i_{tlk,g}(\vec{r}) = \frac{1}{\psi_{lk,g}(\vec{r})}\int_{E_g}^{E_{g-1}} dE\sigma^i_t(E)\psi_{lk}(\vec{r},E)$$

$$\psi_{lk}(\vec{r},E) = \int_{4\pi} d\Omega \overline{Y}_{lk}(\Omega)\psi(\vec{r},E,\vec{\Omega})$$

$$\sigma^i_{xg}(\vec{r}) = \frac{1}{\psi_{0g}(\vec{r})}\int_{E_g}^{E_{g-1}} dE\sigma^i_x(E)\psi_0(\vec{r},E) \quad (x = c, f)$$

$$\psi_{lk,g}(\vec{r}) = \int_{E_g}^{E_{g-1}} dE\psi_{lk}(\vec{r},E)$$

$$\nu\sigma^i_{fg}(\vec{r}) = \frac{1}{\psi_{0g}(\vec{r})}\int_{E_g}^{E_{g-1}} dE\nu^i(E)\sigma^i_f(E)\psi_0(\vec{r},E)$$

$$\chi^i_{g'g}(\vec{r}) = \frac{1}{\nu\sigma^i_{fg'}(\vec{r})\psi_{0g'}(\vec{r})}\int_{E_g}^{E_{g-1}} dE\int_{E_{g'}}^{E_{g'-1}} dE'\chi^i(E'\to E)\nu^i(E')\sigma^i_f(E')\psi_0(\vec{r},E')$$

$$\sigma^i_{slk,g'g}(\vec{r}) = \frac{1}{\psi_{lkg'}(\vec{r})}\int_{E_g}^{E_{g-1}} dE\int_{E_{g'}}^{E_{g'-1}} dE'\sigma^i_{sl}(E'\to E)\psi_{lk}(\vec{r},E')$$

- Consistent P_n correction for total and within-group scattering XS

$$\sigma^i_{tg}(\vec{r}) = \sigma^i_{t0,g}(\vec{r})$$

$$\tilde{\sigma}^i_{slk,g'g}(\vec{r}) = \sigma^i_{slk,g'g}(\vec{r}) + [\sigma^i_{t0,g}(\vec{r}) - \sigma^i_{tlk,g}(\vec{r})]\delta_{gg'}$$

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