

# NUCL 511 Nuclear Reactor Theory and Kinetics

**Lecture Note 10** 

**Prof. Won Sik Yang** 

Purdue University
School of Nuclear Engineering

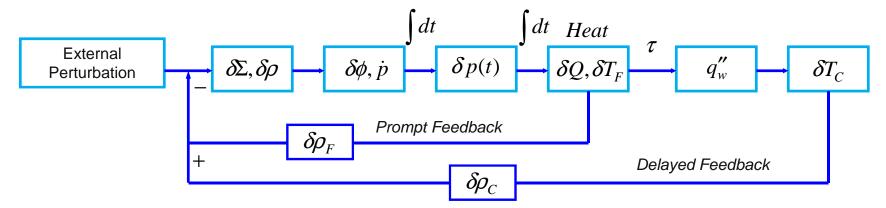




### Reactivity Feedback Mechanism

- What is reactivity feedback?
  - Reactivity change induces changes in thermal condition which can affect back to the reactivity 

    thermal feedback
- Feedback Mechanism



- Prompt feedback
  - Occurs immediately due to fuel temperature change
- Delayed feedback
  - Heat conduction to coolant takes time
  - Caused by coolant density change (thermal expansion) which changes moderation or leakage



## **Doppler Broadening**

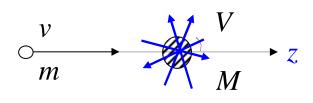
- The laboratory cross section should be defined to agree with the observed reaction rate.
  - The cross section is determined by the relative speed, as opposed to the laboratory speed of neutron
  - The Doppler broadened cross section will not generally be the same as the cold cross section
- If  $P(\vec{V})d\vec{V}$  is the probability at temperature T that a nucleus (or atom) has velocity  $\vec{V}$  within  $d\vec{V}$  about  $\vec{V}$ , the observed reaction rate that a neutron with velocity  $\vec{V}$  will collide with a nucleus is

$$R(v,T) = v\sigma(v,T) = \int [v_r \sigma(v_r,0)] P(\vec{V}) d\vec{V}$$

If the velocity distribution of the target nuclei is isotropic, we have

$$P(\vec{V})d\vec{V} = \frac{1}{4\pi}P(V)dVd\mu d\varphi$$

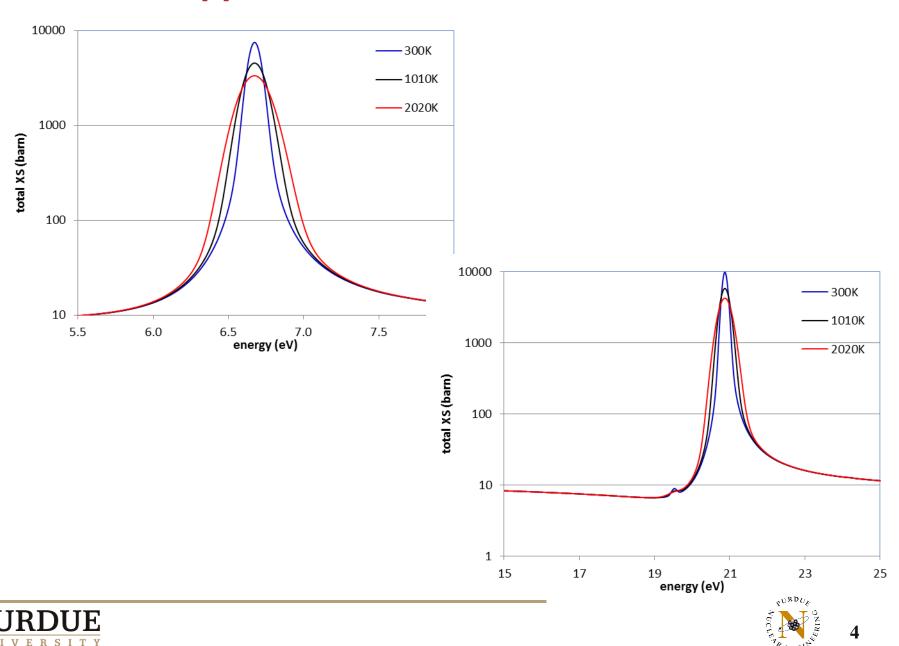
$$\sigma(v,T) = \frac{1}{2v} \int_{-1}^{1} d\mu \int_{0}^{\infty} dV[v_{r}\sigma(v_{r},0)]P(V)$$







# **Doppler Broadened U-238 Total XS**



#### **Free Gas Model**

The relative speed can be written as

$$v_r = |\vec{v} - \vec{V}| = (v^2 + V^2 - 2vV\mu)^{1/2}$$

The Jacobian transformation from the cosine of scattering angle to the relative speed is given by

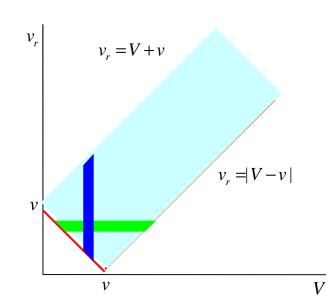
$$d\mu = v_r dv_r / vV$$

■ Changing the integration variable from  $\mu$  to  $\nu_r$ , we have

$$\sigma(v,T) = \frac{1}{2v^2} \int_{|v-V|}^{v+V} [v_r \sigma(v_r, 0)] v_r dv_r \int_0^{\infty} P(V) \frac{dV}{V}$$
$$= \frac{1}{2v^2} \int_0^{\infty} [v_r \sigma(v_r, 0)] v_r dv_r \int_{|v-v_r|}^{v+v_r} P(V) \frac{dV}{V}$$

For the Maxwellian monatomic (or free) gas model, the distribution of nuclei speed is given by

$$P(V)dV = 4\pi \left(\frac{a}{\pi}\right)^{3/2} V^2 e^{-aV^2} dV; \quad a = \frac{M}{2kT}$$





## **Doppler Broadened Cross Section**

The Doppler broadened cross section is obtained as

$$\sigma(v,T) = \frac{2a^{3/2}}{\sqrt{\pi}v^2} \int_0^\infty [v_r \sigma(v_r, 0)] v_r dv_r \int_{|v-v_r|}^{v+v_r} V e^{-aV^2} dV$$

$$= \frac{a^{1/2}}{\sqrt{\pi}v^2} \int_0^\infty [v_r \sigma(v_r, 0)] v_r \left[ e^{-a(v-v_r)^2} - e^{-a(v+v_r)^2} \right] dv_r$$

This can be rewritten in terms of energy as

$$\sigma(E,T) = \frac{\alpha^{1/2}}{2\sqrt{\pi}E} \int_0^\infty \left[\sqrt{E_r}\sigma(E_r,0)\right] \left[e^{-\alpha(\sqrt{E}-\sqrt{E_r})^2} - e^{-\alpha(\sqrt{E}+\sqrt{E_r})^2}\right] dE_r$$

$$E = \frac{1}{2}mv^2; \quad E_r = \frac{1}{2}mv_r^2; \quad \alpha = \frac{2a}{m} = \frac{M}{mkT} = \frac{A}{kT}$$

For large  $\alpha \sqrt{EE_r}$  (~ AE/kT), the second exponential can be ignored, compared to the first

$$\sigma(E,T) = \frac{\alpha^{1/2}}{2\sqrt{\pi}E} \int_0^\infty \left[\sqrt{E_r}\sigma(E_r,0)\right] e^{-\alpha(\sqrt{E}-\sqrt{E_r})^2} dE_r$$



# Single Level Breit-Wigner Formula

Doppler broadened cross section

$$\sigma(E,T) = \frac{1}{\Delta\sqrt{\pi E}} \int_{-\infty}^{\infty} [\sqrt{E_r} \sigma(E_r)] e^{-[(E_r - E)/\Delta]^2} dE_r$$

$$\Delta = \left(\frac{4kTE}{A}\right)^{1/2}$$
 (Doppler width)

Single level Breit-Wigner formula

$$\sigma_a(E_r) \approx \sigma_0 \frac{\Gamma_a}{\Gamma} \frac{1}{1+w^2} \quad (a=\gamma, f)$$

$$\sigma_n(E_r) \approx 4\pi a^2 + \sigma_0 \frac{\Gamma_n}{\Gamma} \frac{1}{1+w^2} + \sigma_0 ka \frac{2w}{1+w^2}$$

$$w = \frac{E_r - E_0}{\Gamma / 2}$$

$$\sigma_0 = \frac{4\pi}{k^2} g_J \frac{\Gamma_n}{\Gamma}$$
 (resonance peak),  $k = \frac{2\pi}{\lambda}$  (wave number)





0.5

2

## **Doppler Broadened Line Shape Functions**

Doppler broadened cross sections

$$\sigma_{a}(E,T) = \sigma_{0} \frac{\Gamma_{a}}{\Gamma} \sqrt{\frac{E_{0}}{E}} \psi(x,\xi), \quad (a = \gamma, f)$$

$$\sigma_{n}(E,T) = 4\pi a^{2} + \sigma_{0} \frac{\Gamma_{n}}{\Gamma} \psi(x,\xi) + 2\sigma_{0} ka \chi(x,\xi)$$

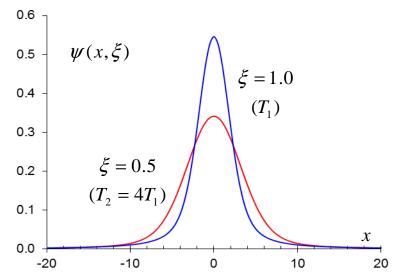
$$x = \frac{E - E_{0}}{\Gamma/2}, \quad \xi = \frac{\Gamma}{\Delta}, \quad \sqrt{\frac{E_{0}}{E}} \approx 1$$

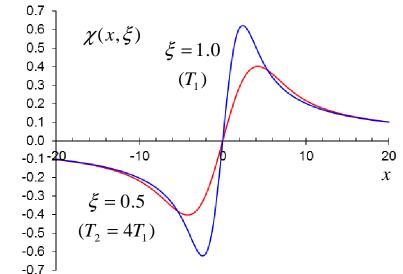
 Symmetric and anti-symmetric Doppler broadened line shape functions

$$\psi(x,\xi) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{1}{1+w^2} \exp\left[-\frac{\xi^2}{4}(x-w)^2\right] dw$$

$$\chi(x,\xi) = \frac{\xi}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{w}{1+w^2} \exp\left[-\frac{\xi^2}{4}(x-w)^2\right] dw$$

$$\sqrt{E_r} \approx \sqrt{E_0}$$









#### **Psi-Chi Functions**

Doppler broadened line shape functions can be represented as convolution integrals of Lorentzian L and Gaussian kernel G as

$$\psi(x,\xi) = \int_{-\infty}^{\infty} L(w)G(x-w;\xi)dw = L(x)*G(x,\xi)$$

$$\chi(x,\xi) = \int_{-\infty}^{\infty} 2wL(w)G(x-w,\xi)dw = [2xL(x)]*G(x,\xi)$$

$$L(x) = \frac{1}{1+x^2} \text{ (natural line shape)}, \quad G(x,\xi) = \frac{\xi}{2\sqrt{\pi}} \exp\left(-\frac{\xi^2}{4}x^2\right) \text{ (pure Doppler shape)}$$

At a very low temperature ( $\xi = \Gamma_t / \Delta >> 1$ ), the Doppler broadened line shapes reduce to the natural line shapes

$$\lim_{\xi \to \infty} \psi(x, \xi) = \int_{-\infty}^{\infty} L(w)\delta(x - w)dw = L(x), \quad \lim_{\xi \to \infty} \psi(x, \xi) = \int_{-\infty}^{\infty} 2wL(w)\delta(x - w)dw = 2xL(x)$$

At a very high temperature ( $\xi = \Gamma_t / \Delta << 1$ ), the Doppler broadened line shapes reduce to the pure Doppler shapes

$$\lim_{\xi \to 0} \psi(x,\xi) = \frac{\xi\sqrt{\pi}}{2} \int_{-\infty}^{\infty} \delta(t) \exp\left[-\frac{1}{4}(\xi x - t)^2\right] dt = \pi G(x,\xi)$$

$$\lim_{\xi \to 0} \chi(x, \xi) = \sqrt{\pi} \int_{-\infty}^{\infty} \delta(t) t \exp\left[-\frac{1}{4} (\xi x - t)^2\right] dt = 0$$



## **Self-Shielding Factor**

Group-averaged cross section is computed

$$\sigma_{xg}^{i}(T,\sigma_{b}) = \frac{\int_{g} \sigma_{x}^{i}(E,T)\phi_{i}(E,T,\sigma_{b})dE}{\int_{g} \phi_{i}(E,T,\sigma_{b})dE} = \frac{\int_{g} \sigma_{x}^{i}(E,T)C(E)/[\sigma_{b} + \sigma_{t}^{i}(E,T)]dE}{\int_{g} C(E)/[\sigma_{b} + \sigma_{t}^{i}(E,T)]dE}$$

■ Traditional J-integral approach for SLBW resonances

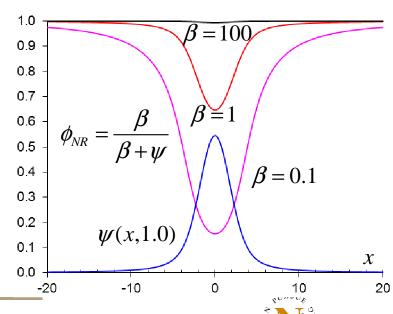
$$I_k^i(T, \sigma_b) = C \int \frac{\sigma_t^i(E, T)}{\sigma_b + \sigma_t^i(E, T)} dE = C \frac{\Gamma}{2} \int \frac{\sigma_0^i \psi(x, \xi)}{\sigma_b + \sigma_0^i \psi(x, \xi)} dx = C \Gamma J(\beta, \xi)$$

$$J(\xi, \beta) = \int_0^\infty \frac{\psi(x, \xi)}{\beta + \psi(x, \xi)} dx, \quad \beta = \frac{\sigma_b}{\sigma_o^i}$$

$$\lim_{\beta \to \infty} J(\xi, \beta) = \frac{1}{2\beta} \int_{-\infty}^{\infty} \psi(x, \xi) dx = \frac{\pi}{2\beta}$$

Self-shielding factor

$$f(T, \sigma_b) = \frac{\sigma(T, \sigma_b)}{\sigma(0, \infty)} \approx \frac{2\beta}{\pi} J(\xi, \beta)$$

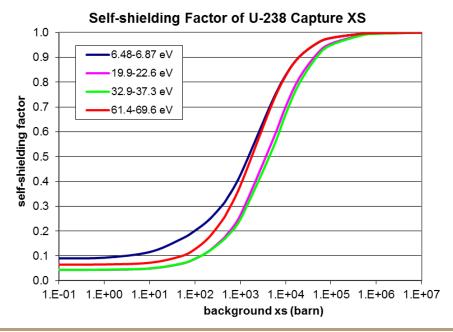


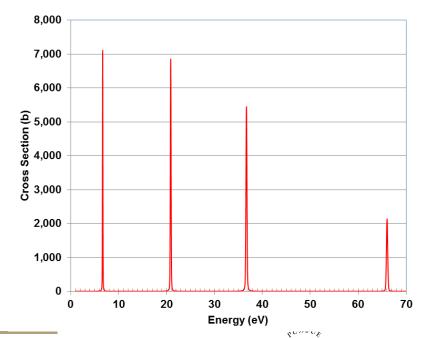
## **Background Cross Section Dependence**

- Absorption decreases with increasing background cross section
  - Self-shielding factor increases

$$\frac{\partial J}{\partial \beta} = -\int_{0}^{\infty} \frac{\psi(x,\xi)}{\left[\beta + \psi(x,\xi)\right]^{2}} dx < 0$$

$$\frac{\partial f}{\partial \beta} = \frac{\partial}{\partial \beta} \left[ \frac{2\beta}{\pi} J \right] = \frac{2}{\pi} \left[ J + \beta \frac{\partial J}{\partial \beta} \right] = \int_{0}^{\infty} \left[ \frac{\psi(x, \xi)}{\beta + \psi(x, \xi)} \right]^{2} dx > 0$$







## **Temperature Dependence**

- Absorption increases with increasing temperature
  - Reactivity decreases and thus the Doppler coefficient is negative

$$\frac{\partial J}{\partial \xi} = \int_{0}^{\infty} \frac{\beta}{\left[\beta + \psi(x,\xi)\right]^{2}} \frac{\partial \psi}{\partial \xi} dx = \int_{0}^{x_{\xi}} f(x) \frac{\partial \psi}{\partial \xi} dx - \int_{x_{\xi}}^{\infty} f(x) \left| \frac{\partial \psi}{\partial \xi} \right| dx$$

$$< f(x_{\xi}) \int_{0}^{x_{\xi}} \frac{\partial \psi}{\partial \xi} dx - f(x_{\xi}) \int_{x_{\xi}}^{\infty} \left| \frac{\partial \psi}{\partial \xi} \right| dx = f(x_{\xi}) \int_{0}^{\infty} \frac{\partial \psi}{\partial \xi} dx = 0$$

$$\frac{\partial}{\partial T} J(\xi, \beta) = \frac{\partial J}{\partial \xi} \frac{d\xi}{dT} = -\frac{\Gamma_{t}}{2} \left( \frac{A}{4kE} \right)^{1/2} T^{-3/2} \frac{\partial J}{\partial \xi} > 0$$

$$0.3$$

$$\frac{\partial}{\partial \xi} dx = 0$$

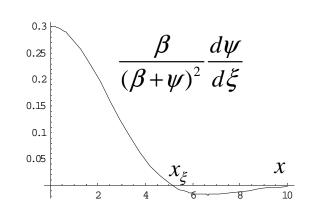
$$0.3$$

$$0.2$$

$$0.15$$

$$0.05$$

$$0.05$$



- Self-shielding effect decreases with increasing temperature
  - Self-shielding factor increases

$$\frac{\partial f}{\partial T} = \frac{\partial}{\partial \xi} \left[ \frac{2\beta}{\pi} J \right] \frac{d\xi}{dT} = -\frac{\beta \Gamma_t}{\pi} \left( \frac{A}{4kE} \right)^{1/2} T^{-3/2} \frac{\partial J}{\partial \xi} > 0$$

### **Low Temperature**

- At a very low temperature,  $\xi >> 1$  and the Doppler broadened line shape reduces to the natural line shape.
- In this case, the J function and self-shielding factor become

$$\lim_{\xi \to \infty} J(\xi, \beta) = \int_0^\infty \frac{L(x)}{\beta + L(x)} dx = \frac{1}{\beta} \int_0^\infty \frac{dx}{(1 + \beta^{-1}) + x^2} = \frac{\pi}{2\beta (1 + \beta^{-1})^{1/2}}$$

$$f(\infty, \beta) = \left(\frac{\beta}{1+\beta}\right)^{1/2} \approx \begin{cases} \sqrt{\beta} & \text{for small } \beta \\ 1 - \frac{1}{2\beta} & \text{for large } \beta \end{cases}$$

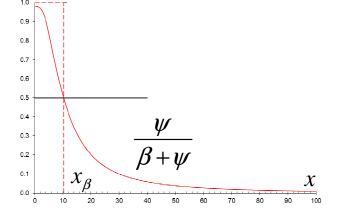
- This eliminates the temperature dependence from the self-shielding factor.
  - The resonance is un-broadened and has its maximum height.
  - This leads to the strongest self-shielding and thus to the smallest value of the self-shielding factor



## **High Resonances at Low Energies**

- For high resonances ( $\beta$  <<1) at low energies, the integrand of the J function is close to 1 for the high part of the resonance. The integrand decreases on the resonance wings, becomes equal to 1/2 where  $\psi(x_{\beta}, \xi) = \beta$ , and vanishes asymptotically.
  - The J integral can be approximated by the area of the rectangle of height 1 and width  $x_{\beta}$
  - $x_{\beta}$  can be determined from the approximation for dominating Doppler broadening

$$\beta = \psi(x_{\beta}, \xi) \approx \frac{\sqrt{\pi}\xi}{2} \exp\left(-\frac{\xi^2}{4}x_{\beta}^2\right)$$



$$J(\xi, \beta) \approx x_{\beta} \approx \frac{2}{\xi} \sqrt{\ln \frac{\sqrt{\pi} \xi}{2\beta}} \propto \frac{1}{\xi} \propto \sqrt{T}, \quad \frac{\partial}{\partial T} J(\xi, \beta) \propto \frac{1}{\sqrt{T}}$$

Since high resonances dominate in the 1/E spectrum of thermal reactors, the resonance integral in thermal reactors depends on temperature through a  $\sqrt{T}$  term, and the Doppler coefficient has a temperature dependence as  $1/\sqrt{T}$ 



## Low Resonances at High Energies

■ For resonances which are much lower than the potential cross section,  $\beta >> \psi$  and hence the J function can be approximated as

$$J(\xi,\beta) = \int_0^\infty \frac{\psi}{\beta + \psi} dx = \frac{1}{\beta} \int_0^\infty \frac{\psi}{1 + (\psi/\beta)} dx \approx \frac{1}{\beta} \int_0^\infty \psi \left(1 - \frac{\psi}{\beta}\right) dx = \frac{\pi}{2\beta} - \frac{\pi}{4\beta^2} \psi(0,\sqrt{2}\xi)$$

For low resonances at high energies, Doppler broadening generally dominates ( $\xi >> 1$ ) and hence

$$\psi(x,\xi) \approx \pi G(x,\xi) = \frac{\xi\sqrt{\pi}}{2} \exp\left(-\frac{1}{4}\xi^{2}x^{2}\right) \implies \psi(0,\sqrt{2}\xi) \approx \sqrt{\frac{\pi}{2}}\xi = \frac{\sqrt{\pi}\Gamma_{t}}{\sqrt{2}} \left(\frac{A}{4kE}\right)^{1/2} \frac{1}{\sqrt{T}}$$

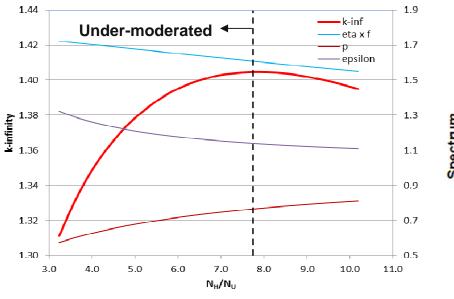
$$\frac{\partial}{\partial T} J(\xi,\beta) \approx \left(\frac{\pi}{2}\right)^{3/2} \frac{\Gamma_{t}}{4} \left(\frac{A_{t}}{4kE}\right)^{1/2} \left(\frac{N_{t}\sigma_{m}^{k}}{\Sigma_{p}}\right)^{2} T^{-3/2}$$

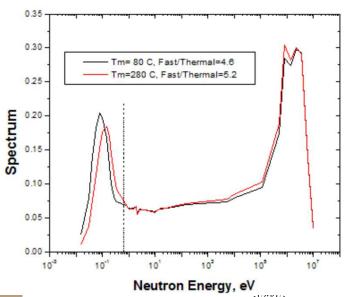
- In the very hard spectrum of small fast reactors, the temperature dependence is determined by the  $T^{-3/2}$  contributions of the high energy resonances.
- In the relatively soft neutron spectra of large ceramic fueled fast reactors, it is between the two limiting cases of high resonances  $(T^{-3/2})$  and low resonances  $(T^{-1/2})$ .
- A simple analytical evaluation of the medium height resonances is not feasible. A numerical evaluation of the high, medium, and low resonance contributions to the Doppler coefficient in large fast reactors yields an approximate proportionality to T<sup>-1</sup>



#### **Moderator Effects**

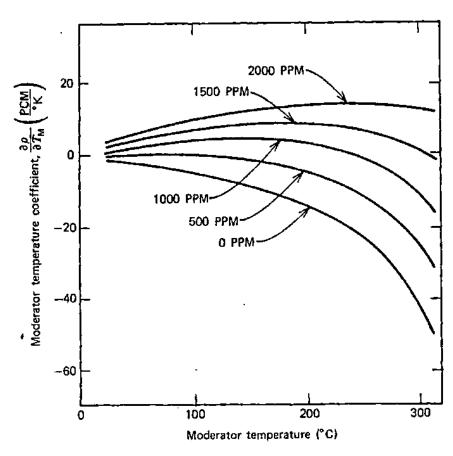
- Change in moderator temperature induces changes in moderator density and scattering kernel
- Fuel-to-moderator ratio in under-moderated region for negative MTC
  - $T_m \uparrow \Rightarrow d_m \downarrow \Rightarrow$  spectrum hardening  $\Rightarrow$  resonance absorption  $\uparrow \Rightarrow \rho \downarrow$
  - In PWR,  $d_m \downarrow \Rightarrow$  boron concentration  $\downarrow \Rightarrow \rho \uparrow$ 
    - MTC becomes less negative as boron concentration increases
    - Boron concentration is limited since MTC can be positive at very high concentration (2500 ppm)



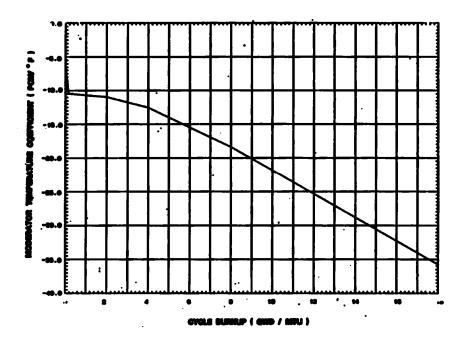




#### **Moderator Temperature Coefficient of PWR**



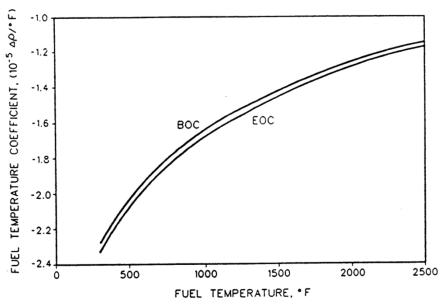
 MTC becomes more positive with boron concentration because of larger reduction in poison content from reduced density (increased temperature)

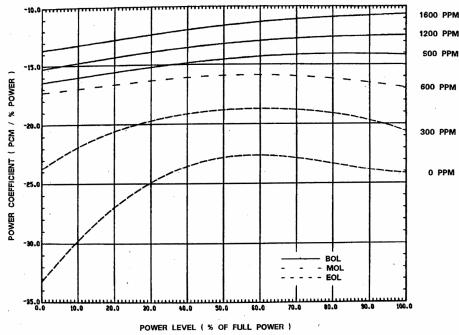


- MTC becomes more negative with burnup primarily because of the reduction in boron concentration with burnup
- Large negative value would be limiting for a cold water injection incidence
- MTC becomes more negative with control rod insertion because of hardened neutron spectrum and increased leakage



#### **Fuel Temperature and Power Coefficients of PWR**



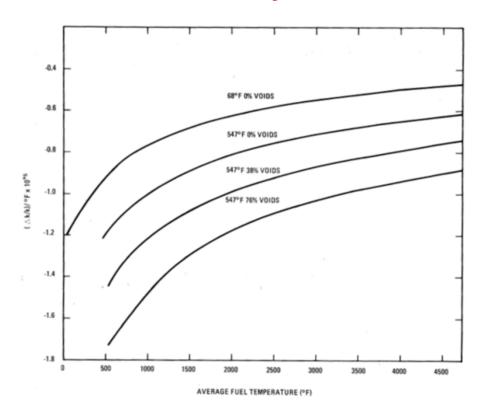


- Magnitude of fuel temperature coefficient decreases with increasing fuel temperature
- Becomes more negative with burnup because of Pu-240 contribution

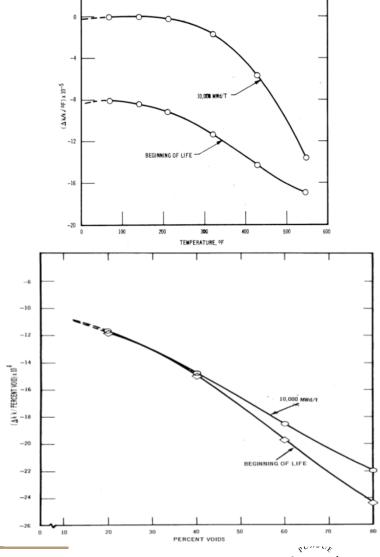
- Power reactivity coefficient must be negative under all operating conditions
- Coefficient becomes more negative with burnup because of the MTC contribution



### **Reactivity Feedback Coefficients of BWR**



- Coolant temperature coefficient is valid in the core heat-up range
- Void coefficient is valid in the power range of operation





## Reactivity Feedback Coefficients of SFR

- The reactivity coefficients and kinetic parameters further define the physics of system
  - Response to a variety of perturbations
- Feedback coefficients are computed for a specific design (geometric and material) configuration
  - Typically evaluated for BOEC and EOEC compositions
- Typical set of whole-core reactivity coefficients
  - Delayed neutron fraction and prompt neutron lifetime
  - Coolant density coefficient and void worth
  - Fuel and structural Doppler coefficient
  - Fuel and structural worth distributions
  - Axial expansion
  - Radial expansion
  - Control rod driveline expansion
- Hummel and Okrent Reactivity Coefficients in Large Fast Power Reactors, ANS, 1970 is a good reference for underlying physics



## **Neutron Balances of Radial and Axial Expansions**

	Base Case	Radial Expansion		Axial Expansion	
	balance	balance	Δρ (%)	balance	Δρ (%)
Fission source	100.00	100.00		100.00	
(n,2n) source	0.18	0.18		0.18	
Absorption	68.89	68.93	-0.04	69.06	-0.17
Leakage	31.54	32.16	-0.63	31.69	-0.16
Radial	17.49	17.72	-0.23	17.65	-0.15
Axial	14.05	14.45	-0.40	14.04	0.01
Sum			-0.67		-0.33

- To first order, radial expansion is an axial leakage effect, and axial expansion is a radial leakage effect
- Because the height is the shorter dimension (more axial than radial leakage), the radial expansion coefficient is more negative
- Axial expansion also give absorption effect from control rod insertion



## **Coolant Density and Void Coefficients**

- Spectral effect
  - Reduced moderation as sodium density decreases
  - In fast regime, this is a positive reactivity effect
    - From Pu-239 excess neutrons and threshold fission effects
- Leakage effect
  - Sodium density reduction allows more neutron leakage
  - This is a negative reactivity effect in the peripheral regions
- Capture effect
  - Sodium density decrease results in less sodium capture
  - This is a relatively minor effect
- Coolant density coefficient is computed by first-order perturbation theory to evaluate small density (temperature variation) impacts
- Void worth is evaluated using exact perturbation theory to account for shift in flux distribution for voided condition
  - In general, 10% more positive than the first-order density worth



## **Sodium Void Worth by Components (\$)**

		Capture	Spectral	Leakage	Total
1000 MWt ABR	ВОС	0.5	9.1	-5.2	4.4
(startup metal core)	EOC	0.5	9.9	-5.5	4.9
250 MWt ABTR	вос	0.4	6.4	-5.8	1.0
(startup metal core)	EOC	0.4	6.6	-5.8	1.1

- Flowing sodium was voided in active and above-core regions
- Void worth tends to increase with core size
- However, difficult to conceive transient situations that reach boiling
  - Low pressure system
  - More than 300°C margin to boiling
  - Other feedbacks are negative, inhibiting this temperature increase
- Extensive report on void worth reduction Khalil and Hill, NS&E, 109 (1995)

