On the effect of the resonant dependent scattering kernel for heavy isotopes

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Topics

- **Introduction**
- **The resonance dependent scattering kernel**
- **Experiments**
- **Angular distribution**
- **Solid state effects**

The Transport equation and the scattering kernel term

$$\frac{1}{v}\frac{\partial f(E,r,\Omega,t)}{\partial t}+\Omega\cdot\nabla f(E,r,\Omega,t)+\left[\Sigma_s(E)+\Sigma_a(E)\right]f(E,r,\Omega,t)=$$

$$=\int_{\Omega'}\int_0^{\infty}\Sigma(E'\rightarrow E;\Omega'\rightarrow\Omega)\,f(E',r,\Omega',t)\,d\Omega'\,dE'+S(E,r,\Omega,t)$$

How good can we calculate the scattering kernel term for heavy isotopes?

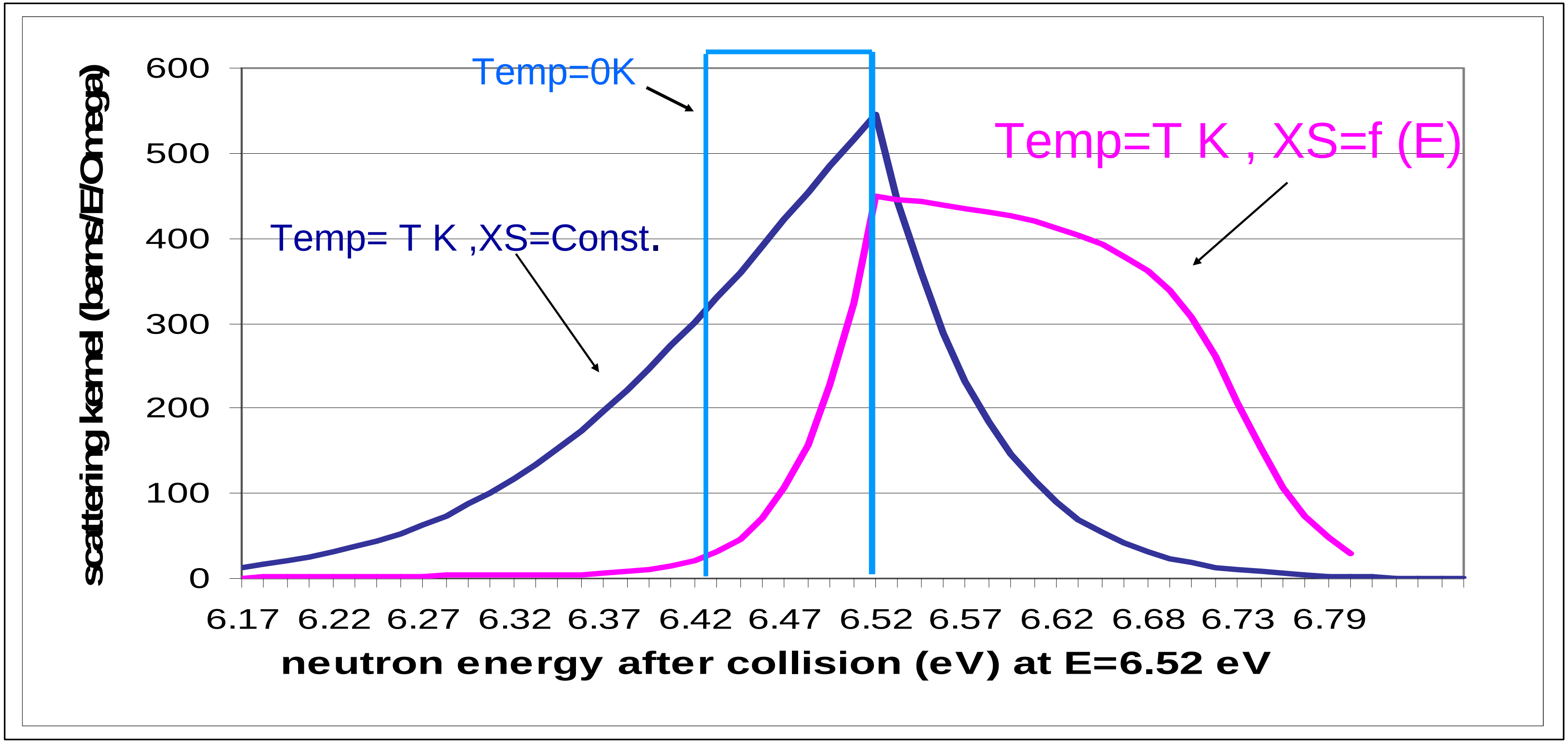
- The resonant scattering cross section is temperature and energy dependent

BUT → The resonant scattering kernel is (usually) used at 0K and energy independent.

What are the consequences of this approximation?

MCNP Scattering Kernel Treatment: “Sampling the target velocity”

- **“If the energy of the neutron is greater than 400KT and the target is not Hydrogen the velocity of the target is set to Zero”** **(Asymptotic kernel)**



The double differential scattering kernel

$$\sigma_S^T(E \to E', \Omega \to \Omega') \; ; \; \sigma_s = \sigma_s(E)$$

- Ann. Nucl. Energy. 1998 25 p 209
- Ann. Nucl. Energy. 2004 31 p 9

- This kernel can be solved numerically in reasonable time and was implemented in THERMR.

- The new kernel is mathematically consistent and in accordance with the BROADR module (Doppler broadening) of NJOY

- Formatted probability tables can be prepared for MCNP calculations as it is done for light isotopes.

IDEAL GAS KERNEL: ENERGY DEPENDENT $\sigma_s(E_\tau)$

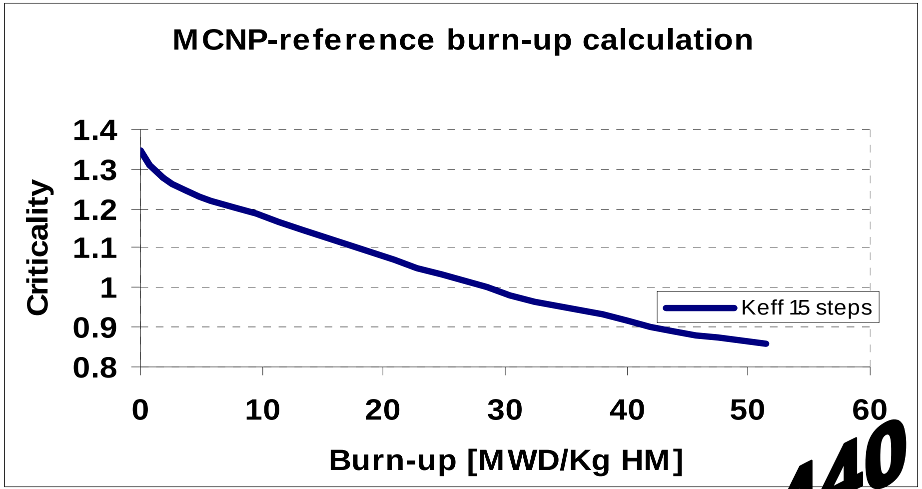
$$\sigma_s^T(E \to E', \hat{\Omega} \to \hat{\Omega}') =$$

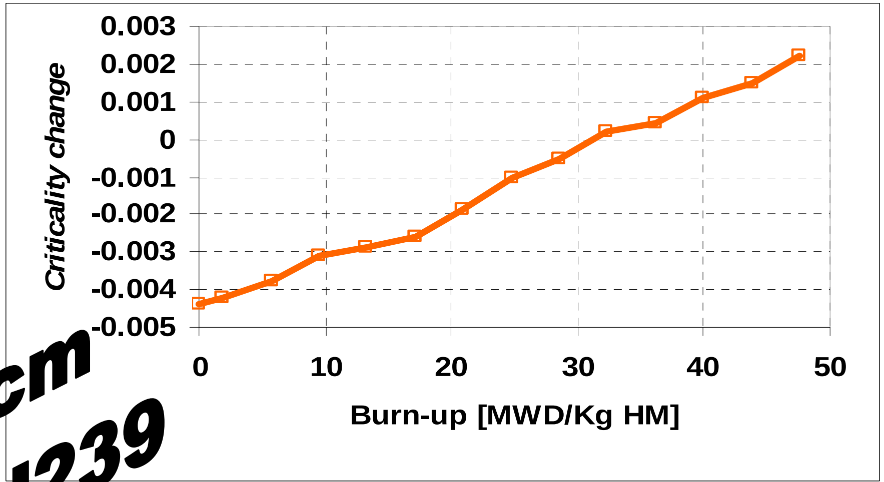
$$\frac{1}{4\pi E}\sqrt{\frac{A+1}{A\pi}}\int_{\epsilon_{max}}^{\infty} d\xi \int_{\tau_0(\xi)}^{\tau_1(\xi)} d\tau$$

$$\left[\frac{(\xi+\tau)}{2}\right]\left(\frac{A+1}{A}\right)^2 \sigma_s\left[\left(\frac{A+1}{A^2}\right)\frac{[\xi+\tau]^2}{4}k_B T\right]$$

$$\exp\left\{v^2 - \left[\frac{(\xi+\tau)^2}{4A} + \frac{(\xi-\tau)^2}{4}\right]\right\}\left[\frac{\epsilon_{max}\epsilon_{min}(\xi-\tau)^2}{B_0 \sin\hat{\varphi}}\right]$$

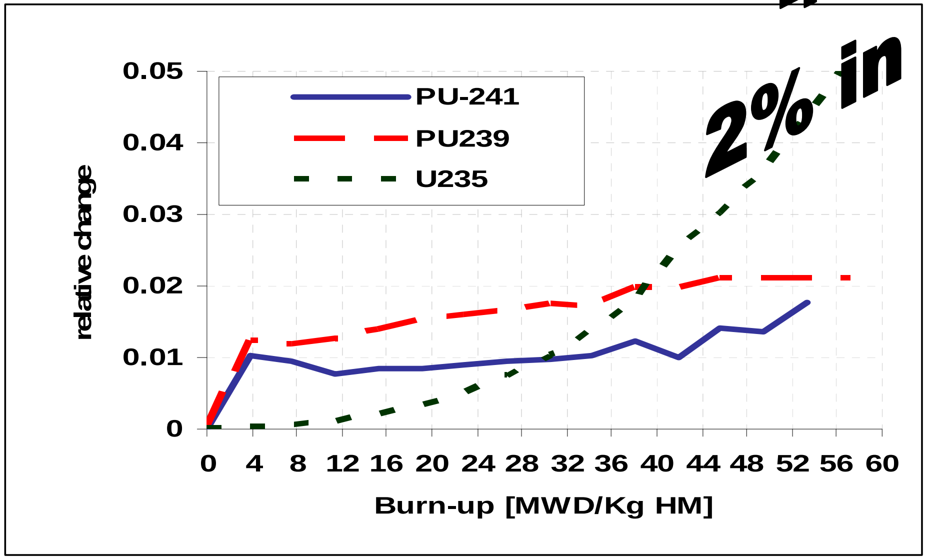
Impact of the modified kernel on criticality and fuel cycle
Pin cell (1200 K)

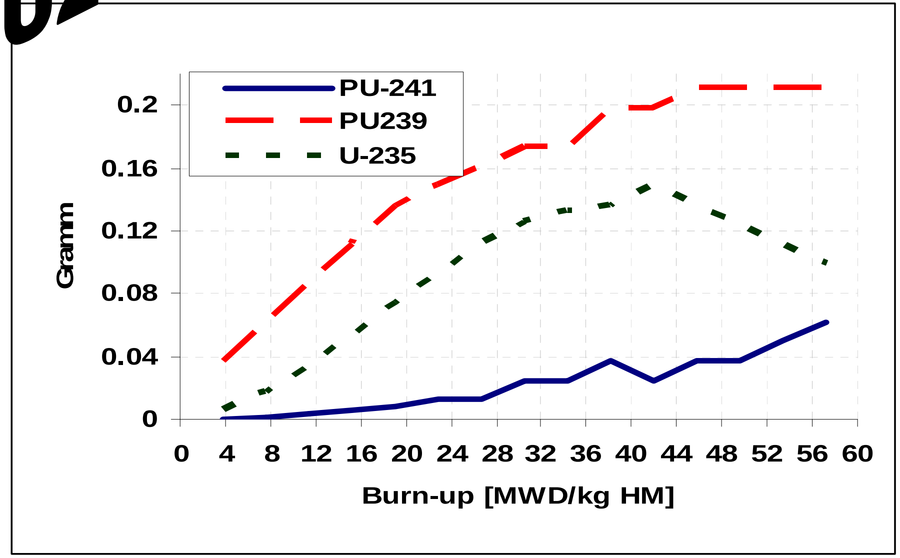




440 pcm

2% in PU239





Experiments

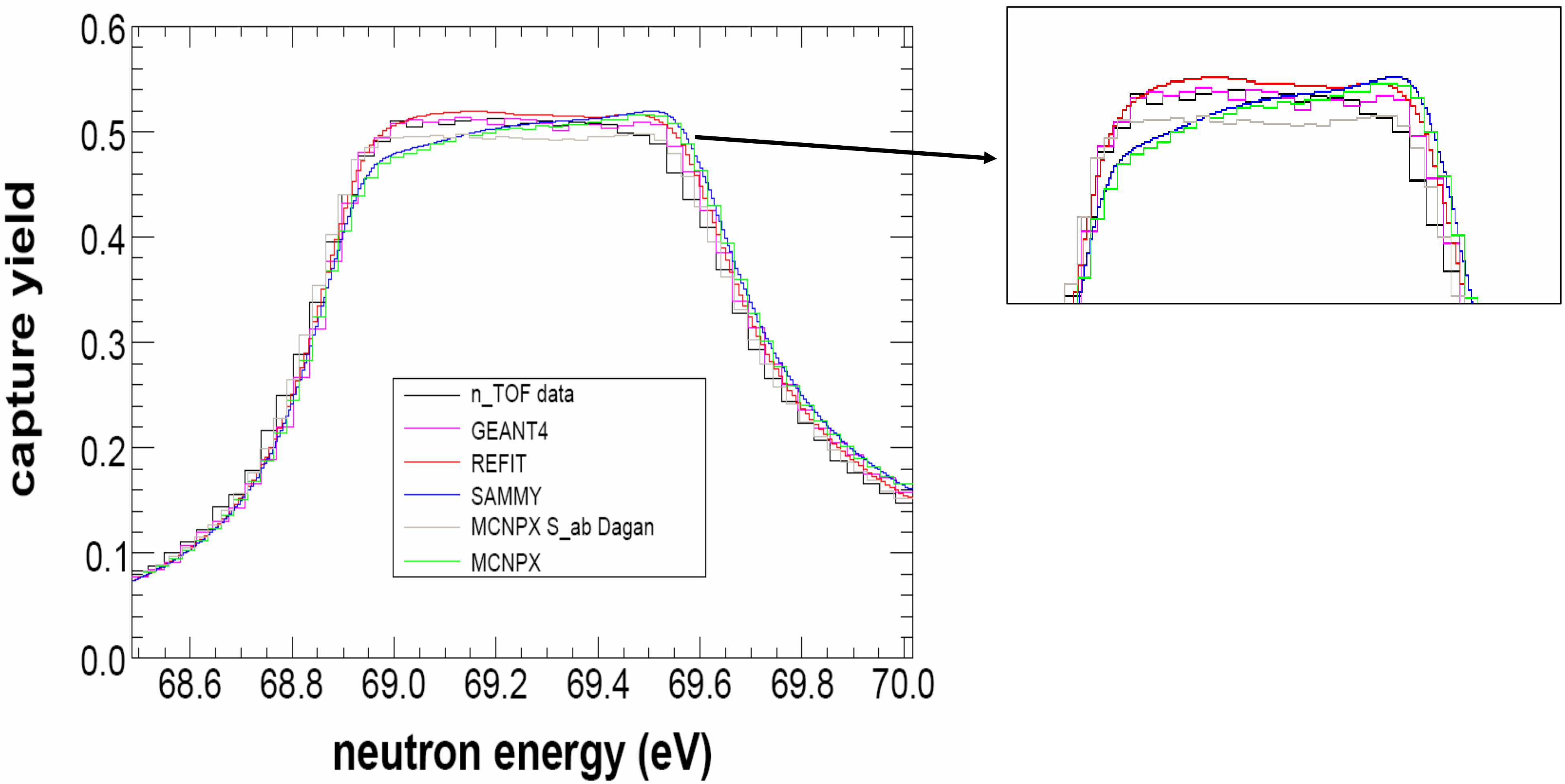
Global:

- The trend of the new scattering kernel to increase the absorption in U238 resonances does not comply with the „needs“ of criticality measurements
- Deviations of the inventory of burned up fuel in comparison with the conventional numerical models

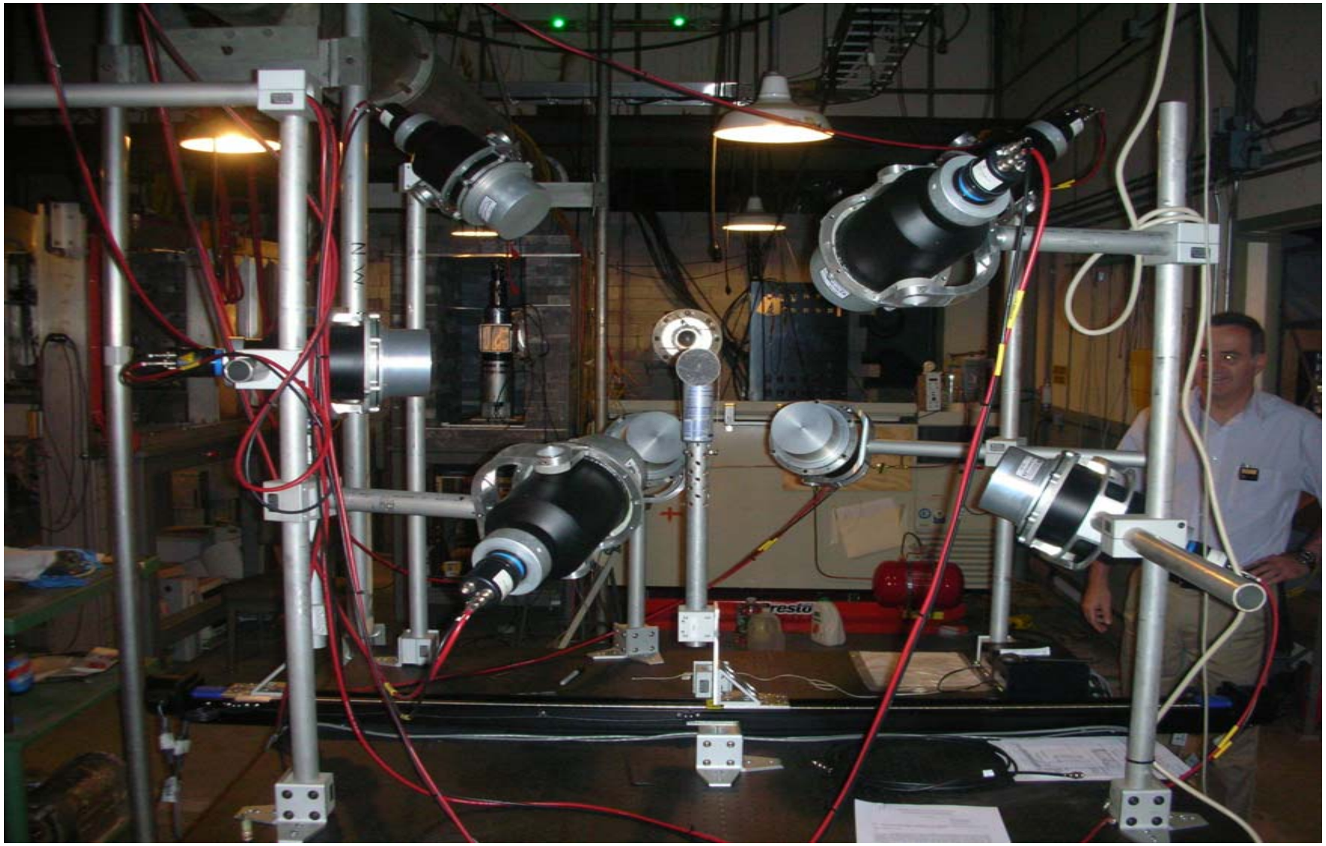
Dedicated Measurements:

- Pu240 (resonance at 1.02 eV)
- TH232 (resonance at 69.24 eV)
- U238? (RPI)

n-TOF Measurements TH232 (CERN 2007) comparison of all codes



RPI facility for the angle distribution measurements



The Transport equation and the scattering kernel term

$$\frac{1}{v}\frac{\partial f(E,r,\Omega,t)}{\partial t} + \Omega \cdot \nabla f(E,r,\Omega,t) + \left[\Sigma_s(E) + \Sigma_a(E)\right] f(E,r,\Omega,t) =$$

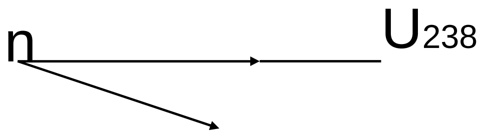
$$= \int_{\Omega'} \int_0^{\infty} \Sigma(E' \to E; \Omega' \to \Omega) f(E',r,\Omega',t)\, d\Omega' dE' + S(E,r,\Omega,t)$$

$$\Sigma(E' \to E; \Omega' \to \Omega) \equiv \Sigma(E' \to E; \theta, \varphi \to \theta', \varphi')$$

The azimuth angle

The asymptotic solution (0 K , XS=Const.):

the azimuth angle is completely independent



$$\frac{E'}{E} = \frac{A^2 + 2A\mu_{cm} + 1}{(A+1)^2} \qquad (1a)$$

$$\mu_{lab}^{0K} = \frac{A\mu_{cm} + 1}{(A^2 + 2A\mu_{cm} + 1)^{1/2}} \qquad (1b)$$

The Sab solution (T k , XS=Const.):

the azimuth angle exists implicitly

$$\sigma(E \to E', \vec{\Omega} \to \vec{\Omega}') = \frac{\sigma_b}{4\pi k_B T}\sqrt{\frac{E'}{E}} < \delta(\beta + \alpha + 2\vec{v}_q \cdot \vec{V} >_T \qquad (2)$$

$$\alpha = (E + E' - 2\sqrt{EE'}\mu_{lab})/(Ak_B T) \quad ; \quad \beta = \frac{E' - E}{K_B T}$$

The angular distribution (2)

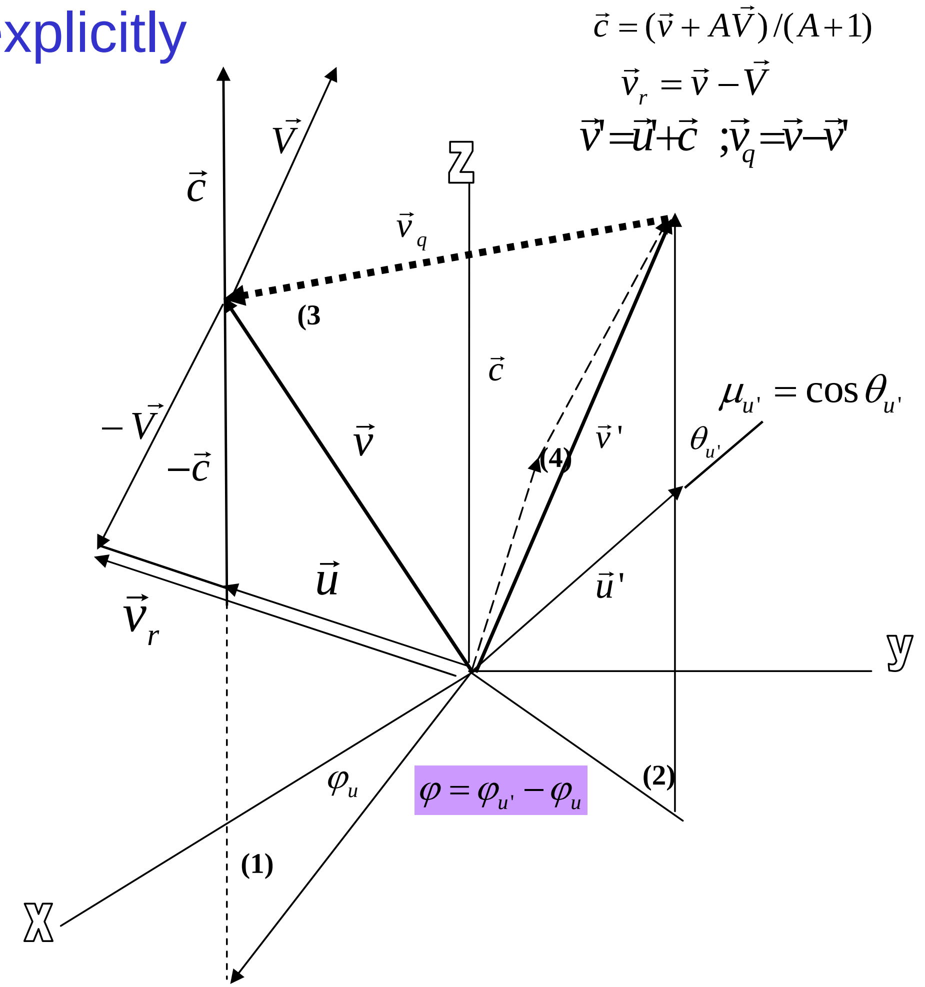
The new resonance dependent
Sab solution (T k , XS=f(E):
the azimuth angle exists explicitly

$$\mu_{cm} = \frac{A_0^{'} + B_0^{'} \cos\varphi}{4uu'c^2} \quad ;$$

$$\mu_{Lab} = \frac{C_0^{'} + B_0^{'} \cos\varphi}{4vv'c^2}$$

$$A_0^{'} = (v^2 - c^2 - u^2)\left[(v')^2 - c^2 - (u')^2\right]; C_0^{'} = (v^2 + c^2 - u^2)\left[(v^{'})^2 + c^2 - (u')^2\right]$$

$$B_0^{'} = \sqrt{\left[(u+c)^2 - v^2\right]\left[(u'+c)^2 - (v')^2\right]\left[v^2 - (u-c)^2\right]\left[(v')^2 - (u'-c)^2\right]}$$



The azimuth angle of the scattering process where the CoM velocity is parallel to the Z axis

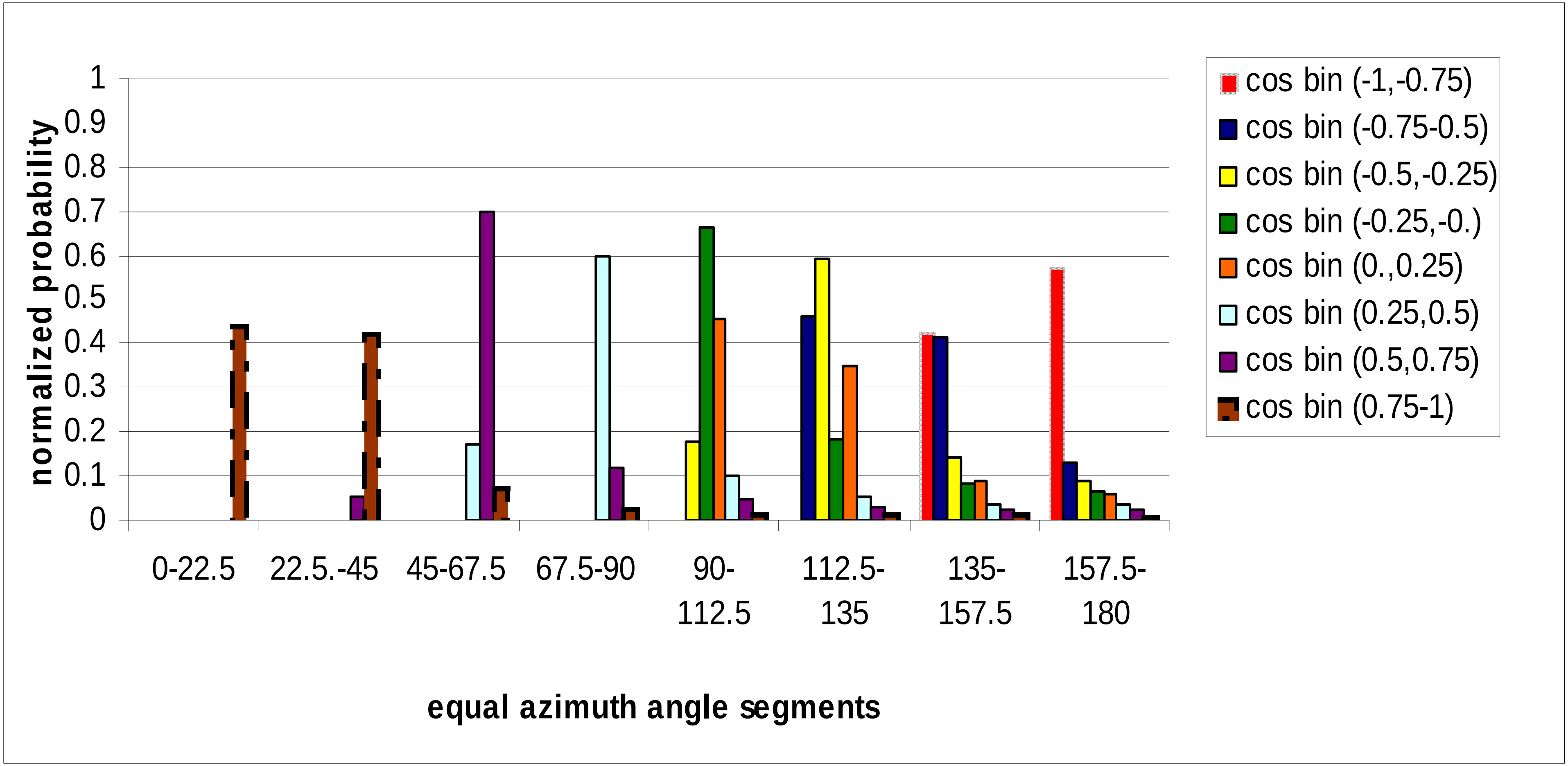
$$\sigma_s^T(E \to E', <\Delta\varphi(\Delta\hat{\mu}_0^{lab})>) = \sqrt{\frac{A+1}{A\pi}} \frac{\exp(E/k_B T)}{E} \int_0^{\infty} dt \{t\sigma_s^{tab}(E_r, 0)\} \exp\frac{t^2}{A}$$

$$\left[H(t_+ - t) H(t - t_-) \int_{\varepsilon_{\max - t}}^{t+\varepsilon_{\min}} dx\, e^{-x^2} + H(t - t_+) \int_{t-\varepsilon_{\min}}^{t+\varepsilon_{\min}} dx\, e^{-x^2} \right]$$

$$2(\varphi_1 - \varphi_2) \frac{P(u, \hat{\mu}_0^{CM})}{2\pi} / \Delta\mu_0^{lab}$$

$$t = u\sqrt{(A+1)} \quad ; x = c\sqrt{(A+1)} \quad ; \varepsilon = v\sqrt{(A+1)} ; \varepsilon' = v'\sqrt{(A+1)}$$

The pronounced anisotropic azimuth angle distribution probability for neutrons scattering with U238 at 1000K



Scattering kernel from 6.9 eV to 6.9 eV for 8 polar cosine bins

The azimuth treatment in MCNP

- Classical two body kinetic namely the 0 K collision approximation below 400KT
- Two options in MCNP are based on interaction with nuclides which behave like a free gas as far as their thermal agitation is concerned:

  1) “Sampling the Velocity of the Target nucleus” (SVT) method.

  2) Pre-prepared probability tables based on constant cross section or resonant cross section.
- In (1) the polar and azimuth angle are sampled. The velocity of the scattered neutron is calculated.
- In (2) the polar and azimuth angle and the velocity are sampled.

Inconsistency between the two approaches within MCNP

Resonance Scattering in a Solid in view of the free gas treatment

- In considering the problem of resonance scattering, we have to try to understand why Shamaoun and Summerfield (1990) and Naberejnev (2001) come to apparently different conclusions concerning the relationship of scattering in a solid to that in a free gas (when the short collision time approximation is used, as is appropriate for higher energy resonances and higher temperatures).
- Both begin their studies of resonance scattering in a solid by starting from the equations developed by Trammell (Phys. Rev. 1966) and further developed by Trammell and Chalk and by Word and Trammell (Phys. Rev.1981).

The expression for the incoherent scattering cross-section is given by Naberejnev and also by Shamaoun and Summerfield as the "four point correlation function" (given here in Naberejnev's notation).

$$\frac{d^2\sigma_R}{d\Omega dE} = \frac{\upsilon}{2\pi}\left(\frac{\Gamma_n}{2k_i}\right)^2\left(\frac{E_f}{E_i}\right)^{1/2}\int_{-\infty}^{\infty} dT \exp(+iET)\int_0^{\infty} dt \exp[a(t)]\int_0^{\infty} dt'$$
$$\times \exp[a^*(t')] \times W(T, t, t'),$$

$$W(T, t, t') = \left\langle \exp\left[-i\vec{k}_i\vec{r}(T-t')\right]\exp\left[i\vec{k}_f\vec{r}(T)\right]\right.$$
$$\left.\exp\left[-i\vec{k}_f\vec{r}\right]\exp\left[i\vec{k}_i\vec{r}(-t)\right]\right\rangle.$$

$$a(t) = -i(E_r - E_i - i\Gamma/2)t.$$

Naberejnev's Method:
A CONSTANT CROSS SECTION APPROACH

- Naberejnev neglects the dependence on t and t' in the third factor in the expression for the scattering and makes the short collision time approximation to treat some other terms. It appears that this partly decouples the cross-section for compound nucleus formation from the energy of the scattered neutron.
- Naberejnev makes calculations and concludes:

At a temperature of 300 K the free gas model gives an upscattering probability at E_i = 6.52 eV of 45.69% and at E_i = 7.2 eV, of 16.5%. The MUPA formalism predicts a smaller probability for a neutron to gain energy after the collision at the lower energy, an upscattering probability equal to 22.6% and 16.5% at the higher energy. (However, 7.2 eV is well above the 6.67eV resonance at 300K)

- *Naberejnev's results are similar to the values obtained for constant cross section scattering kernel calculated directly by free gas model (Dagan ANE 2005)*

SUMMARY

- The improved scattering kernel treatment for U238 has a noticeable effect on the fuel cycle:
  - different criticality values
  - PU239 Inventory increased by ~2%.
  - U235 Inventory is increased accordingly.
  - Doppler increase at BOC: About 13% between 800 K and 1200 K

- Direct TOF measurements confirm (so far) the new scattering kernel based on the free gas model

- RPI dedicated experiments are needed for the validity of the anticipated angular distribution based on energy dependent cross section.
- Inconsistency within the MCNP scattering treatment
- The azimuth angle cannot be calculated in isotropic independent manner.
- The chemical binding effects for heavy isotopes are currently reviewed.