The role of k0 constants as part of the general nuclear data-base

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Topics

• Objectives
• Neutron spectrum
  – Thermal
  – Epithermal
  – Fast
• Reaction rates
• Activation equations
• Cadmium filter
• Nuclear constants for NAA
• Conclusions
Objectives

- $k_0$ NAA is acknowledged as a powerful analytical technique
- Evolution – not revolution
- Explore limitations
- Propose improvements (backward-compatible)
- Feedback to nuclear data evaluations
Neutron spectrum (thermal reactors)

- Thermal: Maxwellian: \( E e^{-E/kT} \)
- Epithermal: \( 1/E \)
- Fast: fission spectrum: \( \sqrt{E} e^{-E/kT} \)

Spectrum spans many orders of magnitude
Makes comparisons difficult
Typical thermal reactor spectrum

\( \Phi(E) \)
Lethargy spectrum

Definition

\[ u = \log E \ ; \psi(u) = E \varphi(E); \int \psi(u) \, du = \int \varphi(E) \, dE \]

Features:

- Takes out the strong energy dependence spanning many orders of magnitude
- Log scale in energy = lethargy scale
- Linear scale in \( \psi \) implies that area under the curve is proportional to the flux integral
Same spectrum in lethargy scale

Lethargy Spectrum

- Mxw_1
- 1/E
- Fis.Mxw
Epithermal and fast spectrum

• Deviations from $1/E$ shape parametrised by $\alpha$

$$\varphi(E) = \frac{1}{E^{1+\alpha}}$$

– This is usually a good approximation

• Fast spectrum can be represented by a fission Maxwellian distribution

$$\varphi_f = \sqrt{E} e^{-E/kT}$$

– Note difference from thermal Maxwellian
– Falls of rapidly above 2 MeV
Idealised spectrum (full range)

Lethargy Spectrum

- Mxw_1
- $1/E$
- Fis.Mxw
- $\alpha + 0.02$
- $\alpha - 0.02$
Real reactor spectra (TRIGA Mark-II)
Reaction rate

• Parametrised by:
  – $\sigma(E)$ property of the irradiated material
  – $\phi(E)$ property of the irradiation facility

$$A = K \int_0^\infty \sigma(E) \phi(E) \, dE$$
Reaction rate (cont.)

In terms of average parameters:

\[ A = K \langle \sigma \rangle \langle \varphi \rangle \]

\[ \langle \varphi \rangle = \int \varphi(E)dE ; \quad \langle \sigma \rangle = \frac{\int \sigma(E)\varphi(E)dE}{\int \varphi(E)dE} = \frac{A}{\langle \varphi \rangle} \]

(Average quantities are defined to preserve reaction rate exactly)
Reaction rate

• Split:
  – No loss of generality (mathematical identity)

\[ A = K \int_0^{E_{Cd}} \sigma(E)\varphi_{th}(E) dE \]

\[ + K \int_{E_{Cd}}^{E_h} \sigma(E)\varphi_e(E) dE + K \int_{E_{Cd}}^{\infty} \sigma(E)\varphi_f(E) dE \]

– \( \varphi_{th}(E) \)  
  thermal Maxwellian with \( 1/E \) tail

– \( \varphi_e(E) \)
  \( 1/E^{1+\alpha} \), drops to zero near \( E_h \)

– \( \varphi_f(E) \)
  fast fission spectrum
Activation equation (per atom)

\[ A = K\{\varphi_{th}\sigma_0 g^* G_{th} + \varphi_e [I G_e + hJ]\} \]

– Choose \( K \) such that \( \varphi_e = 1 \)
– \( hJ \) is a new term describing fast fission
– \( G_x \) are the self-shielding factors
– With above convention we recognize \( \varphi_{th} = f \)
Hence:

\[ A = K\{f \sigma_0 g^* G_{th} + I G_e + hJ\} \]

In conventional \( k_0 \) NAA we divide by \( f \sigma_0 \) (implicitly redefining \( K \))
Specific activity ratios

- Flux normalisation constant cancels out
- We introduce $k_0$ factor

\[
\frac{A_a}{A_s} = k_{0,a} \frac{G_{thf} g_a + G_{e,a} Q_a + H_a h}{G_{thf} g_s + G_{e,s} Q_s + H_s h}
\]

\[
k_{0,a} = \frac{M_s \Theta_a P_{\gamma,a} \sigma_{0,a}}{M_a \Theta_s P_{\gamma,s} \sigma_{0,s}}
\]

\[
Q = \frac{I}{\sigma_0}; \quad H = \frac{J}{\sigma_0}
\]
Thermal range

• Thermal:

\[ A_{th} = \langle \sigma_{th} \rangle \langle \varphi_{th} \rangle \]

• For pure \(1/\nu\) absorbers - exact relationship in a pure Maxwellian spectrum

\[ \langle \sigma \rangle = \frac{\sqrt{\pi}}{2} \sigma_0 \]

• Westcott g-factor takes into account deviations from the \(1/\nu\) cross sections

\[ \langle \sigma \rangle = \frac{\sqrt{\pi}}{2} \sigma_0 \, g \]
Thermal Spectrum

Lethargy Spectrum
Generalised Westcott factor

Conventional definition:

\[ g = \frac{\int_0^\infty \sigma(E) \varphi_{mxw}(E) dE}{\sqrt{\frac{\pi}{2}} \sigma_0 \int_0^\infty \varphi_{mxw}(E) dE} = \frac{2 \sigma_{mxw}}{\sqrt{\pi} \sigma_0} \]

Generalised definition:

\[ g^* = \frac{\int_0^{E_{Cd}} \sigma(E) \varphi_{th}(E) dE}{\sqrt{\frac{\pi}{2}} \sigma_0 \int_0^{E_{Cd}} \varphi_{th}(E) dE} = \frac{2 \sigma_{th}}{\sqrt{\pi} \sigma_0} \]
Thermal spectrum (cont.)

- From the reaction rate definition it follows that flux $\langle \varphi_{th} \rangle$ is the integral of thermal spectrum

$$\langle \varphi_{th} \rangle = \int_0^{E_{Cd}} \varphi_{th}(E) dE$$

- Reaction rate

$$A_{th} = g^* \sigma_0 \frac{\sqrt{\pi}}{2} \langle \varphi_{th} \rangle$$

- $\langle \varphi_{th} \rangle$ can be identified as the $f$ factor
- $g^*$ depends on $f$
Thermal spectrum (cont.)

• Missing part of the spectrum
• Implications:
  – Usually small because experimentally one measures $f_g^*$ and not plain $f$
  – Could be important when $g^*$ of measured isotope differs from standard (Au)
  – Depends on the cross sections
Epithermal spectrum

• Ideally, epithermal spectrum is $1/E$
• $K_e = 1$ is set arbitrarily (permissible because we are always considering ratios)
• Epithermal component ($2^{\text{nd}}$ term) is the resonance integral $I_0$
• Parametrisation of deviation by $\alpha$ seems reasonable
• Approximations to determine $I(\alpha)$ are established
Fast spectrum

- New term is being proposed
  \[ A_h = h\sigma_h \]

  - \(\sigma_h\) can be approximated by cross sections measured in a pure fission spectrum
  - \(h\) can be determined from \(^{27}\text{Al}(n,p)\) or \(^{27}\text{Al}(n,\alpha)\), readily available in Al-Au alloy used as standard
Cd factor

- Cd is a well-chosen filter
- Sharp edge near 5.6 eV
- No distinctly strong resonances above thermal

- Issue:
  - In collimated beams total x.s. governs removal
  - In isotropic beams only absorption removes neutrons – needs some consideration in calculating the cadmium factor $F_{cd}$
Cd cross sections

Total and absorption cross-sections for $^{\text{nat}}$Cd (IRDFF)

- $^{\text{nat}}$Cd $t(E)$, total cross-section (IRDFF)
- $^{\text{nat}}$Cd $t(E)$, absorption cross-section (IRDFF)
Cd transmission function
Cd-attenuation – simple model

• Idealised
  \[ t(E) = \begin{cases} 
  0 & E < E_{cd} \\
  1 & E \geq E_{cd} 
\end{cases} \]

• Simplified realistic
  \[ t(E) = \exp(-N_{cd} \ d \ \sigma_{cd}) \]

  \( N \)  number density of Cd

  \( d \)  thickness of Cd
Cd transmission correction factor

- $F_{cd}$ relates “true” resonance integral to reaction rate integral under Cd cover

\[
I = \int_{E_{cd}}^{E_h} \sigma(E)\varphi(E)dE = \frac{1}{F_{cd}} \int_{0}^{\infty} t(E)\sigma(E)\varphi(E)dE
\]

\[
F_{cd} = \frac{\int_{0}^{\infty} t(E)\sigma(E)\varphi(E)dE}{\int_{E_{cd}}^{E_h} \sigma(E)\varphi(E)dE}
\]
Cd-ratio method

\[
R_{cd} = \frac{A}{A_{cd}} = \frac{f g^* G_{th} + Q G_e + Hh}{Q G_e F_{cd} + Hh}
\]

\[
Q = \left[ \frac{g^* f}{R_{cd} F_{cd} - 1} \right] \frac{G_t}{G_e} - \frac{(R_{cd} - 1) Hh}{(R_{cd} F_{cd} - 1) G_e}
\]
Summary and conclusions

- $k_0$, $Q_0$ are composite constants derived from measured activities.
- It is strongly **recommended** to use the corrections suggested in this presentation.
- Measured activity ratios have broader usage (e.g. differential data validation). Please, report what you measured in a publication with as much detail as possible. A template is available: https://www-nds.iaea.org/naa/rcm2/Tasks/spcact_template.inp
• Example: V. Radulovic, et al.: “Measurement of the neutron activation constants $Q_0$ and $k_0$ for the $^{27}\text{Al}(n, \gamma)^{28}\text{Al}$ reaction at the JSI TRIGA Mark II reactor”, J Radioanal Nucl Chem (2013) 298:1791–1800
  – Fission spectrum contribution affects measured $Q_0$ by 4% in a well-thermalized channel 8% in the core.
## Differential data validation

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