V.B.1. User-Supplied Flux for Watt Spectrum Average

For the Watt spectrum average of Eq. (V B.6) with user-supplied flux, it is necessary to evaluate integrals of the form

$$\int_{\alpha}^{\beta} \sigma(E)\,\varphi(E)\,dE \quad , \tag{V B1.1}$$

in which $\sigma(E)$ is given by one of two types of interpolation (defined below), and $\varphi(E)$ is a linear interpolation between energy points provided by the user. That is, the flux has the form

$$\varphi(E) = d + cE \quad , \tag{V B1.2}$$

and the constants d and c are found by setting the flux equal to the given values at two neighboring points. Specifically, if the set of points $\{E_j^{\varphi}, \varphi_j\}$ are given, then for $E_j^{\varphi} \le E \le E_{j+1}^{\varphi}$, these values are found from

$$\varphi_j = d + cE_j^{\varphi} \quad \text{and} \quad \varphi_{j+1} = d + cE_{j+1}^{\varphi} \quad , \tag{V B1.3}$$

which gives

$$c = \frac{\varphi_{j+1} - \varphi_j}{E_{j+1}^{\varphi} - E_j^{\varphi}} \tag{V B1.4}$$

and

$$d = \frac{E_{j+1}^{\varphi}\varphi_j - E_j^{\varphi}\varphi_{j+1}}{E_{j+1}^{\varphi} - E_j^{\varphi}} \quad . \tag{V B1.5}$$

At sufficiently low energies, far below the lowest resonance, the cross section is generally assumed to be $1/V$, where "velocity" V is the square root of the energy E. In this case, we may approximate the cross section between grid points E_k and E_{k+1} by

$$\sigma(E) = \frac{a}{V} + b \quad , \tag{V B1.6}$$

where a and b are given by

$$a = \frac{V_k\,V_{k+1}}{V_{k+1} - V_k}\left(\sigma_k - \sigma_{k+1}\right) \tag{V B1.7}$$

and

$$b = \frac{V_{k+1}\,\sigma_{k+1} - V_k\,\sigma_k}{V_{k+1} - V_k} \quad , \tag{V B1.8}$$

in which we have set

$$\sigma_k = \sigma(E_k) \quad , \quad \sigma_{k+1} = \sigma(E_{k+1}) \quad , \quad V_k = \sqrt{E_k} \quad , \quad \text{and} \quad V_{k+1} = \sqrt{E_{k+1}} \quad . \tag{V B1.9}$$

Inserting Eqs. (V B1.6) and (V B1.2) into the expression (V B1.1) gives

$$
\begin{aligned}
\int_\alpha^\beta \sigma(E)\,\varphi(E)\,dE &= \int_\alpha^\beta \left\{\frac{a}{V}+b\right\}\{d+cE\}\,dE = \int_{\sqrt{\alpha}}^{\sqrt{\beta}} \left\{\frac{a}{V}+b\right\}\left\{d+cV^2\right\} 2VdV \\
&= 2\int_{\sqrt{\alpha}}^{\sqrt{\beta}} \{a+bV\}\left\{d+cV^2\right\} dV \\
&= 2\int_{\sqrt{\alpha}}^{\sqrt{\beta}} \left\{d(a+bV)+c\left(aV^2+bV^3\right)\right\} dV \qquad \text{(V B1.10)} \\
&= 2\left[d\left(aV+\tfrac{1}{2}bV^2\right)+c\left(\tfrac{1}{3}aV^3+\tfrac{1}{4}bV^4\right)\right]_{\sqrt{\alpha}}^{\sqrt{\beta}} \\
&= d\left[2a\left(\sqrt{\beta}-\sqrt{\alpha}\right)+b(\beta-\alpha)\right]+c\left[\tfrac{2}{3}a\left(\beta^{3/2}-\alpha^{3/2}\right)+\tfrac{1}{2}b\left(\beta^2-\alpha^2\right)\right] \quad .
\end{aligned}
$$

Replacing a and b with their values from Eqs. (V B1.7) and (V B1.8) gives

$$
\begin{aligned}
&\int_\alpha^\beta \sigma(E)\,\varphi(E)\,dE = \\
&\quad d\left[2\frac{V_K\,V_{k+1}}{V_k-V_k}\left(\sigma_k-\sigma_{k+1}\right)\left(\sqrt{\beta}-\sqrt{\alpha}\right)+\frac{V_{k+1}\,\sigma_{k+1}-V_k\sigma_k}{V_{k+1}-V_k}(\beta-\alpha)\right] \qquad \text{(V B1.11)} \\
&\quad +c\left[\frac{2}{3}\frac{V_k\,V_{k+1}}{V_{k+1}-V_k}\left(\sigma_k-\sigma_{k+1}\right)\left(\beta^{3/2}-\alpha^{3/2}\right)+\frac{1}{2}\frac{V_{k+1}\,\sigma_{k+1}-V_k\sigma_k}{V_{k+1}-V_k}\left(\beta^2-\alpha^2\right)\right] \quad ,
\end{aligned}
$$

which can be rearranged in terms of coefficients of σ_k as

$$
\begin{aligned}
&\int_\alpha^\beta \sigma(E)\,\varphi(E)\,dE = \\
&\quad \left[d\left\{2V_{k+1}\left(\sqrt{\beta}-\sqrt{\alpha}\right)-(\beta-\alpha)\right\}+c\left\{\tfrac{2}{3}V_{k+1}\left(\beta^{3/2}-\alpha^{3/2}\right)-\tfrac{1}{2}\left(\beta^2-\alpha^2\right)\right\}\right] \\
&\qquad\qquad \times\frac{\sigma_k\,V_k}{V_{k+1}-V_k} \qquad \text{(V B1.12)} \\
&\quad +\left[d\left\{-2V_k\left(\sqrt{\beta}-\sqrt{\alpha}\right)+(\beta-\alpha)\right\}+c\left\{-\tfrac{2}{3}V_k\left(\beta^{3/2}-\alpha^{3/2}\right)+\tfrac{1}{2}\left(\beta^2-\alpha^2\right)\right\}\right] \\
&\qquad\qquad \times\frac{\sigma_{k+1}\,V_{k+1}}{V_{k+1}-V_k} \quad .
\end{aligned}
$$

This is the form used in SAMMY to evaluate the integral, with the limit α given by either $\alpha = E_k$ = point on energy grid for the cross section or $\alpha = E_j^{\varphi}$ = grid point for the flux generation. Similarly β is either $\beta = E_{k+1}$ or $\beta = E_{j+1}^{\varphi}$.

At higher energies, the cross section is no longer $1/V$. In this case, the cross section between grid points is assumed to be of the form

$$\sigma\left(E\right) = a + bE \quad , \tag{V B1.13}$$

where a and b are given by

$$a = \frac{E_{k+1}\,\sigma_k - E_k\,\sigma_{k+1}}{E_{k+1} - E_k} \tag{V B1.14}$$

and

$$b = \frac{\left(\sigma_{k+1} - \sigma_k\right)}{E_{k+1} - E_k} \quad . \tag{V B1.15}$$

Substituting Eqs. (V B1.13) and (V B1.2) into the expression for the integral in Eq. (V B1.1) gives

$$\begin{aligned} \int_\alpha^\beta \sigma\left(E\right)\varphi\left(E\right)dE &= \int_\alpha^\beta \left\{a + bE\right\}\left\{d + cE\right\}dE \\ &= \int_\alpha^\beta \left\{ad + acE + bdE + bcE^2\right\}dE \\ &= \left[adE + \tfrac{1}{2}\left(ac + bd\right)E^2 + \tfrac{1}{3}bcE^3\right]_\alpha^\beta \\ &= ad\left(\beta - \alpha\right) + \tfrac{1}{2}\left(ac + bd\right)\left(\beta^2 - \alpha^2\right) + \tfrac{1}{3}bc\left(\beta^3 - \alpha^3\right) \quad . \end{aligned} \tag{V B1.16}$$

Inserting the expressions for a and b from Eqs. (V B1.14) and (V B1.15) gives

$$\begin{aligned} &\int_\alpha^\beta \sigma\left(E\right)\varphi\left(E\right)dE = \\ &\quad \frac{E_{k+1}\,\sigma_k - E_k\sigma_{k+1}}{E_{k+1} - E_k}\left[d\left(\beta - \alpha\right) + \tfrac{1}{2}c\left(\beta^2 - \alpha^2\right)\right] \\ &\quad + \frac{\left(\sigma_{k+1} - \sigma_k\right)}{E_{k+1} - E_k}\left[\tfrac{1}{2}d\left(\beta^2 - \alpha^2\right) + \tfrac{1}{3}c\left(\beta^3 - \alpha^3\right)\right] \quad . \end{aligned} \tag{V B1.17}$$

Reorganizing gives coefficients of σ_k:

$$\int_\alpha^\beta \sigma(E)\,\varphi(E)\,dE =$$

$$\left\{d\left[E_{k+1}(\beta-\alpha)-\tfrac{1}{2}\left(\beta^2-\alpha^2\right)\right]+c\left[\tfrac{1}{2}E_{k+1}\left(\beta^2-\alpha^2\right)-\tfrac{1}{3}\left(\beta^3-\alpha^3\right)\right]\right\} \times \frac{\sigma_k}{E_{k+1}-E_k} \tag{V B1.18}$$

$$-\left\{d\left[E_k(\beta-\alpha)-\tfrac{1}{2}\left(\beta^2-\alpha^2\right)\right]+c\left[\tfrac{1}{2}E_k\left(\beta^2-\alpha^2\right)-\tfrac{1}{3}\left(\beta^3-\alpha^3\right)\right]\right\} \times \frac{\sigma_{k+1}}{E_{k+1}-E_k} \quad .$$