V.C.1. Energy- or Time-Weighted Averages for Experimental Data

SAMMY's energy-averaged or time-averaged cross section is an average over a specific energy range or time-of-flight range, with no additional weighting. The implementation of this option assumes that the unaveraged cross section has already been "binned," as would occur during the data-collection process. Hence, this option cannot be used for accurate calculation of averaged theoretical cross sections.

The energy-averaged cross section is of the form

$$\bar{\sigma} = \frac{1}{N} \int_{Emin}^{Emax} \sigma\left(E'\right) dE' \quad , \tag{V C1.1}$$

with the normalization N given by

$$N = \int_{Emin}^{Emax} dE' \; = \; Emax - Emin \quad . \tag{V C1.2}$$

Similarly, the time-averaged cross section has the form

$$\bar{\sigma} = \frac{1}{N} \int_{tmin}^{tmax} \sigma\left(E\left(t'\right)\right) dt' \quad , \tag{V C1.3}$$

with the normalization N given by

$$N = \int_{tmin}^{tmax} dt' \; = \; tmax - tmin \quad . \tag{V C1.4}$$

In practice the integrals in Eqs. (V C1.1) through (V C1.4) are replaced by sums over discrete intervals of the form

$$\bar{\sigma} = \frac{1}{N} \sum_{Imin}^{Imax} \sigma_i \, \Delta_i \quad ; \tag{V C1.5}$$

N is given by the same formula with the σ_i term omitted inside the summation.

For energy averaging, the Δ_i are given by

$$\Delta_i = \frac{1}{2}\left[E_{i+1} - E_{i-1}\right] \quad ; \tag{V C1.6}$$

this is equivalent to assuming that the channel endpoints are exactly halfway between the energies specified as channel energy.

For time-average cross sections, the Δ_i are given by the difference between the time at the end of a channel and the time at the beginning. This assumes that the specified experimental energies are stated at the center of the channel, that is, that the time associated with channel *i* is

$$t_i = \sqrt{\frac{m}{2}\frac{L^2}{E_i}} \qquad \text{(V C1.7)}$$

and Δ_i is given by

$$\Delta_i = \frac{1}{2}\left[t_{i+1} - t_{i-1}\right] \quad . \qquad \text{(V C1.8)}$$

In both cases described above, corrections are made to ensure that the range included in the summation does not extend beyond the minimum and maximum energies, which are not likely to be channel boundaries. Note that neither of these approximations is exactly correct when compared to the experimental situation, since the endpoints of the time-of-flight channels are estimated based on center-time information. A more correct procedure would be to use the exact information from the experimental time-of-flight channels; unfortunately such information is not available to the analysis.

To determine the uncertainties associated with $\bar{\sigma}$, we consider a small increment in $\bar{\sigma}$, which can be written as

$$\delta\bar{\sigma} = \frac{1}{N}\sum_j \sum_i \frac{\partial \sigma_i}{\partial u_j}\Delta_i\, \delta u_j \quad , \qquad \text{(V C1.9)}$$

where u_j are the *u*-parameters (see Section IV.C). Squaring this quantity and taking expectation values give the variance on $\bar{\sigma}$ as

$$Var\left(\bar{\sigma}\right) = \left\langle \left(\delta\bar{\sigma}\right)^2 \right\rangle = \frac{1}{N}\sum_i \sum_{i'} \sum_j \sum_{j'} \frac{\partial \sigma_i}{\partial u_j}\frac{\partial \sigma_{i'}}{\partial u_{j'}}\Delta_i\, \Delta_{i'} \left\langle \delta u_j\, \delta u_{j'} \right\rangle \quad . \qquad \text{(V C1.10)}$$

Note that the quantity $\left\langle \delta u_j\, \delta u_{j'} \right\rangle$ is just the parameter covariance matrix $M_{j\,j'}$, which is known from the earlier analysis. The partial derivatives in Eq. (V C1.10) are readily evaluated within SAMMY, and the Δ_i are known. Thus, the uncertainty on the average cross section $\bar{\sigma}$ may be found directly from this equation.

The input needed to use this option is described in Section VI.F.1. Examples are given in test cases tr014 and tr075.