V.D. STELLAR-AVERAGED CAPTURE CROSS SECTIONS

Stellar-averaged capture cross sections* may be generated for nuclear astrophysics applications. These are similar to the Maxwellian average used in reactor applications (see Section V.B on Integral Quantities) but defined in a somewhat different fashion. They are obtained from the stellar reaction rate formula [KW84],

$$\left\langle \sigma(E)\sqrt{E} \right\rangle_{kT} = \int_0^\infty \sigma_{capture}(E)\sqrt{E}\, W(E,kT)\, dE \quad , \qquad \text{(V D.1)}$$

where *W(E,kT)* is the Maxwellian weighting factor

$$W(E,kT) = \frac{2\sqrt{E}\, e^{-E/kT}}{\sqrt{\pi}\,(kT)^2} \quad , \qquad \text{(V D.2)}$$

and the capture cross section $\sigma_{capture}$ is generated from the resolved resonance parameters. The integration is performed numerically in SAMMY, using techniques similar to those described in Section III.A for the broadening integrals.

Energies in the above equations are center of mass. The cross sections generated from resonance parameters are, however, expressed in terms of laboratory energy. The conversion from center of mass to laboratory is

$$E = \frac{M}{m+M} E_{lab} \quad , \qquad \text{(V D.3)}$$

where *m* is the mass of the incident neutron and *M* is the mass of the target nucleus. The integration variable is changed from *E* to E_{lab} before the integral is evaluated.

The numerical integration technique is used to evaluate Eq. (V D.1) instead of the analytical approximation which may be more familiar to nuclear astrophysicists, because the assumptions underlying the analytical approximation are not always valid (see below). SAMMY does, however, calculate and print the approximate value in addition to the numerical result and provides a comparison between the two. (In addition to printing these in the LPT file output, SAMMY also generates an output file SAM16.DAT which contains only the table of stellar averages.)

The assumptions under which the analytical approximation is derived are the following: (1) The function $e^{-E/kT}$ is constant across the width of a resonance. (2) The neutron width $\Gamma_{n\lambda}$ is constant across the width of a resonance. (3) The multilevel Breit-Wigner approximation provides an adequate description for the cross section. (4) The lower-energy limit may be extended from 0 to negative infinity. Under these assumptions, the Maxwellian average has the approximate value

* Only the resolved resonance parameters, not the unresolved, are used in the calculation of Eq. (V D.1). However, point-wise cross sections from ENDF File 3 may be added, as described at the end of this section.

$$\left\langle \sigma(E)\sqrt{E} \right\rangle \cong \frac{\pi^{3/2}}{m}\left(\frac{1}{kT}\right)^2 \sum_{\lambda} e^{-\frac{M}{m+M}\frac{E_\lambda}{kT}} \frac{2g_\lambda \Gamma_{\lambda n}\Gamma_{\lambda\gamma}}{\Gamma_\lambda} + \sqrt{\frac{E_{thermal}}{kT}}\sigma_{capture}\left(E_{thermal}\right) \quad , \tag{V D.4}$$

where the summation includes only those resonances that have positive energies, and the "thermal" energy is somewhat arbitrarily taken to be the lowest energy for which the differential cross sections are calculated. [This is sufficient, since results are the same so long as the energy is low enough that the energy-dependence is $1/V$ (i.e., $1/\sqrt{E}$).]

To generate Maxwellian averages [both the numerically integrated values of Eq. (V D.1) and the analytic approximation values of Eq. (V D.4)], include a line in the INPut file specifying one of the following two statements; note that these are treated identically within SAMMY:

```
MAXWELLIAN AVERAGED capture cross sections are wanted
STELLAR AVERAGED CAPture cross sections are wanted
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It is also necessary to provide an additional input file, the MXW file, containing values for the temperatures at which the calculation is to be performed. See Section VI.F.4, for details.

There are several options in SAMMY for specifying the energy grid on which the numerical integration of Eq. (V D.1) will take place. Because the precision with which the results are calculated may depend upon the method chosen, the user is encouraged to try different options to ensure that the desired accuracy is achieved. The first option is to use an experimental (i.e., user-provided) grid. A better alternative is to begin with the experimental grid, but the user should also specify

```
BROADENING IS WANTED
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and give values for at least one broadening parameter. (This might be considered the "default," since this is what would apply if stellar averages were requested but no other thought was given to the specifics.) If the Doppler temperature is specified, it is used only to calculate an energy grid; the cross sections in the Maxwellian average are of course evaluated at zero temperature.

The purpose of specifying that broadening is wanted is to force SAMMY to choose a sufficiently dense auxiliary grid (see Section III.A) to properly describe the structure in the cross section, and thus to ensure accurate integration. Additionally the user may wish to request extra points added between experimental points (see variable NXTRA in card set 2 of the INPut file, Table VI A.1).

Two other options permit SAMMY to choose the energy grid automatically. The first uses the (NJOY) reconstruct option via the command

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RECONSTRUCT CROSS SEction from resonance parameters
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(This command can be used only with the Reich-Moore approximation.) The other option (which can be used also with Breit-Wigner) begins with a uniformly spaced grid, then adds points as needed to describe the structure. This option is invoked with the command

```
ARTIFICIAL ENERGY GRid is needed
```

The number of energy points in the initial (uniformly spaced) grid is given by variable NEPNTS on card set 2 in the INPut file (Table VI A.1).

In all cases, the user specifies EMIN and EMAX as limits for the differential data. Within those energy limits, SAMMY will generate the capture cross section on the chosen energy grid and use those data points for the numerical integration process. External to those limits (i.e., below EMIN and above EMAX), SAMMY will extrapolate in an appropriate fashion in order to reach the integration limits (0 to infinity). SAMMY will issue warnings if the limits seem too confining (i.e., if the integrand does not approach zero at high energy).

Estimates of the covariance matrix for the stellar-averaged capture cross section may be found by using default specifications for solving Bayes' equations (i.e., by not specifying

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DO NOT SOLVE BAYES EQUATIONS
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in the INPut file) and assigning uncertainties (and possibly correlations) to the flagged parameters. Those uncertainties will then be propagated through the averaging process, and the covariance matrix for the stellar-averaged capture cross section will be generated. Caveat: Only those uncertainties included, either implicitly or explicitly, on the flagged parameters will contribute to the uncertainties on the averages. This may result in an underestimation of the uncertainties on the averages, since not all resonance parameter uncertainties can be included.

Often it is important to include values for the capture cross section at higher energies than those described by the resolved resonance parameters (i.e., in the unresolved resonance region). Currently the only way to accomplish this within SAMMY is to present this data as an ENDF file and include the phrase

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ADD CROSS SECTIONS From endf/b file 3
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in the INPut file. SAMMY will ask for the name of this file immediately following the name of the MXW file. For the numerical integration results, the File-3 values are added directly to the resonance cross section before integration; in this case, the differential data are still extrapolated to zero, but the extrapolation beyond EMAX is based on the File-3 values. For the analytic approximation, the File-3 cross sections are integrated (numerically) separately and the results reported both separately and summed with the approximation results.

Test case tr051 contains examples of the various options described above.