Cross Section Data for Preliminary Calculations

In deriving the multigroup neutron balance equation, the group constants were defined as appropriate averages over the energy domain of interest. The general expressions for the broad group cross sections (see Ref. 1 for specific examples) are valid for any energy group. In general, large cross section processing codes are utilized with available fine group or pointwise cross section libraries to obtain broad group data for use in specific analyses. For rough preliminary estimates of the neutronic performance of a system, however, this formal procedure for obtaining broad group data is usually bypassed.

In practice, many preliminary analyses use either 1-group or 2-group models. One-group theory is an appropriate approximation for modeling fast reactor systems. Predetermined 1-group constants are available for most nuclides of interest and rough estimates of reactor performance can be obtained from these data. For example, Table 6.1 in Lamarsh (Ref. 2) gives some nominal 1-group data for use in preliminary fast reactor studies.

Thermal reactors, on the other hand, typically require the use of two energy groups to adequately model the neutronic behavior of the system. Again, tabulated data are often available for initial rough calculations of reactor performance. For example, Lamarsh tabulates typical fast and thermal cross sections for common moderators in Table 5.3 and Table 5.2, respectively. In addition, thermal data for the average number of neutrons emitted per absorption in the fuel, η_T, are given as a function of temperature in Table 6.3. We will use these data quite extensively in many of the numerical computations performed in this course -- and, for convenience, several of these tables from Ref. 2 have been collected as an Appendix to this set of Lecture Notes.

Obtaining absorption and fission data for the fuel nuclides in thermal systems deserves special mention. Thermally averaged parameters are usually obtained from tabulated 2200 m/s data and the following formulas,

$$\bar{\Sigma}_a(T) = \Sigma_{a2}(T) = \frac{\sqrt{\pi}}{2} g_a(T)\,\Sigma_a(E_o)\left(\frac{T_o}{T}\right)^{1/2} \qquad (1)$$

$$\bar{\Sigma}_f(T) = \Sigma_{f2}(T) = \frac{\sqrt{\pi}}{2} g_f(T)\,\Sigma_f(E_o)\left(\frac{T_o}{T}\right)^{1/2} \qquad (2)$$

where the "bar" notation is consistent with that used in Lamarsh (Ref. 2) for the thermally averaged cross sections and the T refers to the material's absolute temperature (T_o = 293 K). Also, in these expressions, $g_a(T)$ and $g_f(T)$ are the non-1/v factors for absorption and fission (see Table 3.2 in Lamarsh for numerical values, for example) and $\Sigma_a(E_o)$ and $\Sigma_f(E_o)$ are the appropriate macroscopic cross sections evaluated at E_o = 0.0253 eV. These macroscopic data are determined by the material composition (i.e. isotope densities) and the 2200 m/s microscopic cross sections for the individual isotopes. There are several possible sources for 2200 m/s cross sections, including Appendix II in Lamarsh (Ref. 2), the Tables of Nuclear Data at the Japan Nuclear Data Center (JNDC) at http://wwwndc.jaea.go.jp/NuC/index.html (Ref. 4), and from the cross section tables vs. energy within the JANIS program which can be obtained from the www.nea.fr/janis/ website (Ref. 5) [where the listing order, Refs. 2, 4, and then 5, represents an ease-of-use or convenience factor in the author's view -- thus, if Appendix II in Ref. 2 is not available, then I suggest that you use the Ref. 4 online source as your next best option...].

The expressions given here are used quite frequently and it is important to have a good understanding of how they are derived -- in particular, these formulas are based on the assumption that the thermal flux spectrum is given by a Maxwellian distribution. Selecting the absorption cross section as an example, the thermally averaged absorption cross section is given formally as

$$\bar{\Sigma}_a = \frac{\int_T \Sigma_a(E)\phi(E)dE}{\int_T \phi(E)dE} = \frac{1}{\phi_T}\int_T \Sigma_a(E)\phi(E)dE \tag{3}$$

where the T in these expressions implies an integration over thermal energies and ϕ_T is the thermal flux.

From previous discussions concerning 1/v and non-1/v cross sections (see the development in Ref. 3 or consult Chapter 3 in Ref. 2), we know that

$$\int_T \Sigma_a(E)\phi(E)dE = g_a(T)\Sigma_a(E_o)\phi_o \tag{4}$$

where ϕ_o is the 2200 m/s flux. Combining eqns. (3) and (4) gives

$$\bar{\Sigma}_a = g_a(T)\Sigma_a(E_o)\frac{\phi_o}{\phi_T} \tag{5}$$

Now recall that ϕ_o is given by

$$\phi_o = n v_o = n\left(\frac{2E_o}{m}\right)^{1/2} = n\left(\frac{2kT_o}{m}\right)^{1/2} \tag{6}$$

where n is the total neutron density, and ϕ_T is given by

$$\phi_T = \int_T n(E)v(E)dE = \int_T n f(E)v(E)dE \tag{7}$$

Now, if we make the assumption that the thermal flux spectrum, f(E), is given by the thermal Maxwellian distribution function, then we can actually perform the integrations implied in eqn. (7). Recall that $v(E) = \sqrt{2E/m}$ and that the Maxwellian is given by

$$f(E) = \frac{2\pi}{(\pi kT)^{3/2}} E^{1/2} e^{-E/kT} \tag{8}$$

Using these expressions ϕ_T becomes

$$\phi_T = \left[\frac{2\pi n}{(\pi kT)^{3/2}}\right]\left(\frac{2}{m}\right)^{1/2}\int_0^\infty \left[E^{1/2}e^{-E/kT}\right]\left[E^{1/2}\right]dE$$

$$\phi_T = \left[\frac{2\pi n}{(\pi kT)^{3/2}}\right]\left(\frac{2}{m}\right)^{1/2}\int_0^\infty E e^{-E/kT}\,dE$$

$$\phi_T = \left[\frac{2\pi n}{(\pi kT)^{3/2}}\right]\left(\frac{2}{m}\right)^{1/2}(kT)^2 = \frac{2}{\sqrt{\pi}}n\left(\frac{2}{m}\right)^{1/2}(kT)^{1/2} \tag{9}$$

where we have used the following integral result as part of the above manipulations,

$$\int_0^\infty E e^{-E/kT}dE = \frac{e^{-E/kT}}{(1/kT)^2}\left(-\frac{E}{kT}-1\right)\Bigg|_0^\infty = -(kT)^2[0-1] = (kT)^2$$

Note also that we have integrated the thermal flux expression over the range $0 \le E \le \infty$ (instead of just the thermal energy range). This approximation is valid since there is negligible contribution to the overall integral above thermal (about 1 eV) as discussed and illustrated in Ref. 3.

Now, from eqn. (6) and eqn. (9), we have a simple relationship for ϕ_o/ϕ_T, or

$$\frac{\phi_o}{\phi_T} = \frac{\sqrt{\pi}}{2}\left(\frac{T_o}{T}\right)^{1/2} \tag{10}$$

and, putting this result back into eqn. (5) gives the original expression written as eqn. (1). This is the desired thermally averaged absorption cross section. The $\sqrt{\pi}/2$ factor that appears in this expression is the result of averaging with the Maxwellian distribution function. Since the absorption and fission data evaluated at $E_0 = 0.0253$ eV are readily available (as noted above), eqns. (1) and (2) are very convenient for determining the thermal data required in any preliminary hand computations.

Now, for the fast region in thermal systems, the broad group data for the fuel and structure nuclides are not as easy to evaluate. Clearly, the best method is to use a sophisticated code to obtain the desired data. However, for quick hand calculations, this is not feasible, and other less accurate techniques are utilized. The primary phenomena of interest in the fast region are fast fission and resonance absorption, and both effects are tough to quantify without fairly detailed calculations. The most common way to treat these processes in making preliminary calculations is to assume that the fast fission and resonance absorption effects are relatively small and to account for fast fission with the so-called ***fast fission factor*** and to handle resonance absorption with the ***resonance escape probability***. We will discuss these quantities in more detail at a later time as the need arises. However, it is important to note that estimates of these "correction factors" are used in preliminary hand calculations only. In all computer analyses of multidimensional systems, the formal development of broad group constants for both the fast and thermal groups is required.

Before leaving the subject of obtaining cross sections for preliminary analyses, it is important to note that most of the data tabulated in Lamarsh (and included in the Appendices to this set of Lecture Notes) are given for nominal density and room temperature conditions. Since the macroscopic cross section is proportional to the nuclide density, Σ is a direct function of the physical density, ρ. The diffusion coefficient, on the other hand, is inversely proportional to ρ and it is only a weak function of temperature. Based on these considerations, the appropriate relationships for accounting for density and temperature effects in preliminary computations are (from Ref. 2):

$$\bar{\Sigma}_a(\rho,T) = \bar{\Sigma}_a(\rho_o,T_o)\left(\frac{\rho}{\rho_o}\right)\left(\frac{T_o}{T}\right)^{1/2} \tag{11}$$

$$\bar{D}(\rho,T) = \bar{D}(\rho_o,T_o)\left(\frac{\rho_o}{\rho}\right)\left(\frac{T}{T_o}\right)^{m} \quad \text{with} \quad m = \begin{cases} 0.470 \text{ for } H_2O \\ 0.112 \text{ for } D_2O \\ \approx 0 \text{ otherwise (solid moderators)} \end{cases} \tag{12}$$

$$L_T^2(\rho,T) = \frac{\bar{D}(\rho,T)}{\bar{\Sigma}_a(\rho,T)} = L_T^2(\rho_o,T_o)\left(\frac{\rho_o}{\rho}\right)^2\left(\frac{T}{T_o}\right)^{m+1/2} \tag{13}$$

and

$$\tau_T(\rho) = \frac{D_1(\rho)}{\Sigma_{1\to 2}(\rho)} = \tau_T(\rho_o)\left(\frac{\rho_o}{\rho}\right)^2 \tag{14}$$

where τ_T is the thermal neutron age. Note that eqn. (14) has no explicit temperature dependence since both D_1 and $\Sigma_{1\to 2}$ are only weakly dependent on the temperature of the material.

Finally, we note that, for materials with significant non-1/v behavior, the temperature dependence of the non-1/v factors, $g_a(T)$ and $g_f(T)$, needs to be incorporated into any preliminary computational estimates.

Well, the goal of this set of Lecture Notes was simply to collect, in a single location, some comments on how to obtain cross section data for performing preliminary reactor calculations. It should be cautioned that the use of the data mentioned here only gives very approximate results -- but this is often sufficient to get a rough idea of the expected behavior of a given system. Much more detailed procedures are needed to get more accurate data for use in more formal design and analysis studies.

With this cautionary note in mind, the following summary list of data sources should be helpful in obtaining approximate cross sections for subsequent homework exercises in this course (note that, for convenience, many of the referenced data tables from Chapters 3, 5, and 6 in Lamarsh are included in the Appendix at the end of this set of Lecture Notes):

1-group data for fast reactors:

Table 6.1 in Lamarsh

2-group data for thermal reactors:

Table 5.3 in Lamarsh for fast data for moderators

Table 5.2 in Lamarsh for thermal data for moderators

Table 6.3 in Lamarsh for η_T data versus temperature

Table 3.2 in Lamarsh for the non-1/v factors needed in eqns. (1) and (2)

See Refs. 2, 4, or 5 for the 2200 m/s microscopic cross section data needed in eqns. (1) and (2) [note that appropriate homogenized nuclide densities are also usually required here for computation of the nuclide-dependent macroscopic cross sections]. As noted earlier, the JNDC Tables of Nuclear Data (Ref. 4) is a particularly convenient online source for these data.

Use eqns. (11) - (14) to account for the temperature and density dependence of the data (especially for moderators).

Quantifying the fast absorption and fission contributions due to the fuel and structural materials is not easy to do, and this is usually treated in preliminary calculations within the context of the fast fission factor and the resonance escape probability (we will discuss this subject further in a later set of Lecture Notes).

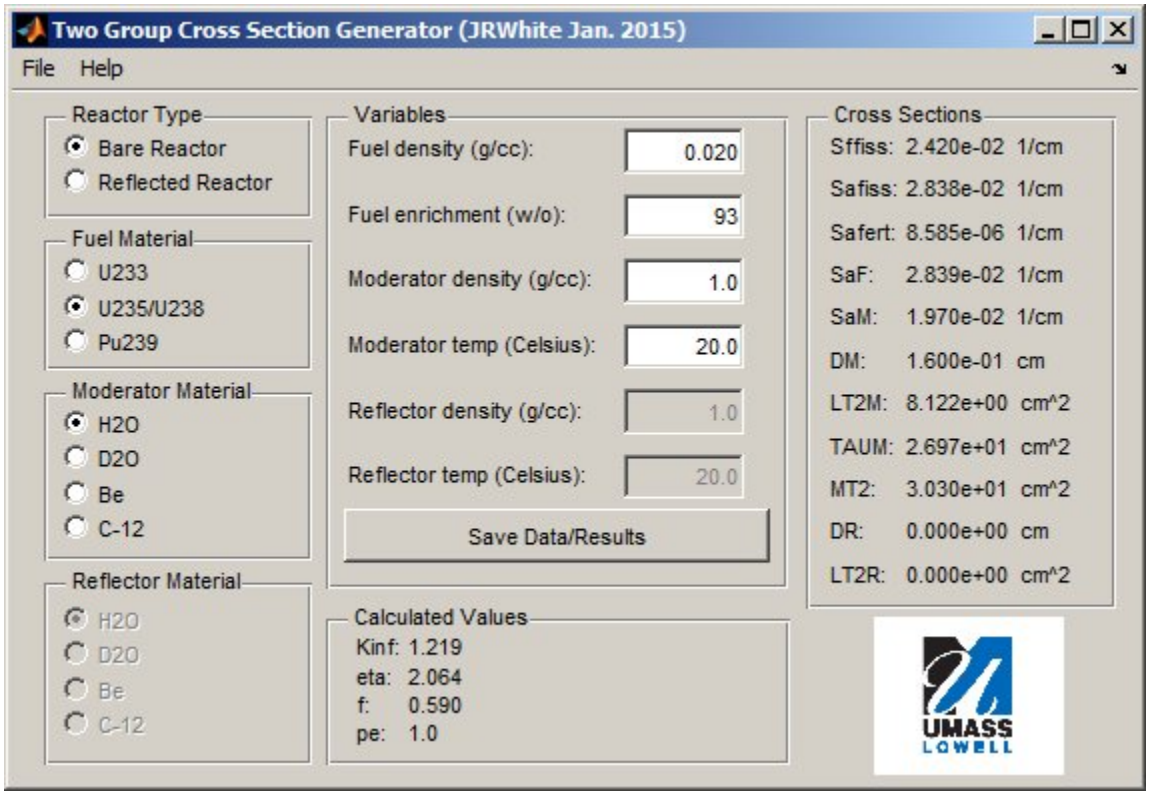

Fig. 1 User interface for the cross_sections_gui code.

In addition to the above summary list of data references, a Matlab graphical user interface, called **cross_sections_gui**, has also been developed to compute many of the thermally averaged cross sections (and other useful auxiliary information) that are needed for performing a variety of analyses for thermal systems. Most of the tabulated data from Lamarsh, as noted above, has been included directly within the **cross_sections_gui** code and, with a simple interface that allows the user to select the materials of interest and specify the appropriate material densities and temperatures, the program can easily compute most of the pertinent macroscopic parameters of interest for the selected core and/or reflector materials [including any density or temperature corrections that may be needed using eqns. (11) – (14)]. The code interface, as shown in the screen shot given in Fig. 1, is simple to use, with the user-specified parameters in the left and central portions of the GUI window, and the computed macroscopic cross sections on the right side of the GUI. In addition, some parameters that allow computation of the infinite multiplication factor, k_∞, for the core material are also contained in the lower central portion of

the window. Note that, even though some of the parameters listed here (f, pε, etc.) have not been formally defined as yet, they have been included within the GUI since they will indeed become very useful for subsequent analyses later in this course. Finally, we note that the central ***Save Data/Results*** button, when pressed, writes all the active information currently displayed on the GUI screen to an ascii text file -- and this can be a very useful documentation tool…

Although the notation used for the code variables within the GUI interface is somewhat obvious, we tabulate the formal correspondence below -- just so there is no chance for any confusion:

Code Variable	Explicit Definition
Sffiss	$\overline{\Sigma}_f$ for fissile fuel (e.g. U235 in a U235/U238 mix)
Safiss	$\overline{\Sigma}_a$ for fissile fuel (e.g. U235 in a U235/U238 mix)
Safert	$\overline{\Sigma}_a$ for fertile fuel (e.g. U238 in a U235/U238 mix)
SaF	$\overline{\Sigma}_{aF} = \overline{\Sigma}_a^{fissile} + \overline{\Sigma}_a^{fertile}$
SaM	$\overline{\Sigma}_a$ for moderator material in core region
DM	$\overline{D}$ for moderator material in core region
LT2M	L_T^2 for moderator material in core region
TAUM	τ_T for moderator material in core region
MT2	$M_T^2 \approx (1-f)L_{TM}^2 + \tau_{TM}$ (migration area for fuel/moderator mix)
DR	$\overline{D}$ for moderator material in reflector region
LT2R	L_T^2 for moderator material in reflector region
Kinf	$k_\infty = \eta_T f p\varepsilon$ (infinite multiplication factor for core material)
eta	η_T (average number of neutrons emitted per thermal absorption in fuel)
f	$f = \overline{\Sigma}_{aF} / \left(\overline{\Sigma}_{aF} + \overline{\Sigma}_{aM}\right)$ (thermal utilization)
pe	pε (product of resonance escape probability and the fast fission factor, where this product is set to unity in the current version of the code since there is no easy way to estimate this quantity [to be discussed later]…)

Many of these quantities are utilized for characterizing the behavior of thermal systems, and these will be needed for several of your assigned homework problems from later in the semester (note that this GUI is NOT appropriate for 1-group fast reactor studies). Thus, access to the **cross_sections_gui** code can help simplify obtaining the data needed for these analyses. In addition, the code can also be used to help validate any hand computations that are performed independent of the **cross_sections_gui** program. Thus, I think you will find that this GUI can be a very useful tool for doing a variety of preliminary reactor and shield design computations…

References

1. J. R. White, "The Multigroup Neutron Balance Equation," part of a series of Lecture Notes for the Nuclear Engineering Program at UMass-Lowell.
2. J. R. Lamarsh and A. J. Baratta, ***Introduction to Nuclear Engineering***, 3rd Edition, Prentice Hall (2001).
3. J. R. White, "Neutron Interactions with Matter (i.e. Neutron Cross Sections)," part of a series of Lecture Notes for the Nuclear Engineering Program at UMass-Lowell.
4. JNDC Tables of Nuclear Data, http://wwwndc.jaea.go.jp/NuC/index.html
5. JANIS program, www.nea.fr/janis/

Appendix -- Cross Section Data Tables directly from Lamarsh (Ref. 2)

TABLE 3.2 NON-1/*V* FACTORS*

	Cd	In	^{135}Xe	^{149}Sm	^{233}U		^{235}U		^{238}U	^{239}Pu	
T,°C	g_a	g_a	$g_a^\dagger$	g_a	g_a	g_f	g_a	g_f	g_a	g_a	g_f
20	1.3203	1.0192	1.1581	1.6170	0.9983	1.0003	0.9780	0.9759	1.0017	1.0723	1.0487
100	1.5990	1.0350	1.2103	1.8874	0.9972	1.0011	0.9610	0.9581	1.0031	1.1611	1.1150
200	1.9631	1.0558	1.2360	2.0903	0.9973	1.0025	0.9457	0.9411	1.0049	1.3388	1.2528
400	2.5589	1.1011	1.1864	2.1854	1.0010	1.0068	0.9294	0.9208	1.0085	1.8905	1.6904
600	2.9031	1.1522	1.0914	2.0852	1.0072	1.0128	0.9229	0.9108	1.0122	2.5321	2.2037
800	3.0455	1.2123	0.9887	1.9246	1.0146	1.0201	0.9182	0.9036	1.0159	3.1006	2.6595
1000	3.0599	1.2915	0.8858	1.7568	1.0226	1.0284	0.9118	0.8956	1.0198	3.5353	3.0079

*Based on C. H. Westcott, "Effective Cross-Section Values for Well-Moderated Thermal Reactor Spectra," Atomic Energy Commission report AECL-1101, January 1962.
†Based on E. C. Smith *et al., Phys. Rev.* **115**, 1693 (1959).

TABLE 5.2 THERMAL NEUTRON DIFFUSION PARAMETERS OF COMMON MODERATORS AT 20°C*

Moderator	Density, g/cm^3	$\overline{D}$, cm	$\overline{\Sigma}_a$, cm^{-1}	L_T^2, cm^2	L_T, cm
H_2O	1.00	0.16	0.0197	8.1	2.85
D_2O†	1.10	0.87	9.3×10^{-5}	9.4×10^3	97
Be	1.85	0.50	1.04×10^{-3}	480	21
Graphite	1.60	0.84	2.4×10^{-4}	3500	59

*Based on *Reactor Physics Constants,* 2nd ed., Argonne National Laboratory report ANL-5800, 1963, Section 3.3.
†D_2O containing 0.25 weight/percent H_2O. These values are very sensitive to the amount of H_2O impurity (see Problem 5.28).

TABLE 5.3 FAST-GROUP CONSTANTS FOR VARIOUS MODERATORS

Moderator	D_1, cm	Σ_1, cm^{-1}	τ_T, cm^2
H_2O	1.13	0.0419	~27
D_2O	1.29	0.00985	131
Be	0.562	0.00551	102
Graphite	1.016	0.00276	368

TABLE 6.1 NOMINAL ONE-GROUP CONSTANTS FOR A FAST REACTOR*

Element or Isotope	σ_γ	σ_f	σ_a	σ_{tr}	ν	η
Na	0.0008	0	0.0008	3.3		
Al	0.002	0	0.002	3.1		
Fe	0.006	0	0.006	2.7	—	—
^{235}U	0.25	1.4	1.65	6.8	2.6	2.2
^{238}U	0.16	0.095	0.255	6.9	2.6	0.97
^{239}P	0.26	1.85	2.11	6.8	2.98	2.61

*From *Reactor Physics Constants*, 2nd ed., Argonne National Laboratory report ANL-5800, 1963.

TABLE 6.3 VALUES OF η_T, THE AVERAGE NUMBER OF FISSION NEUTRONS EMITTED PER NEUTRON ABSORBED IN A THERMAL FLUX, AT THE TEMPERATURE T

T, °C	^{233}U	^{235}U	^{239}Pu
20	2.284	2.065	2.035
100	2.288	2.063	1.998
200	2.291	2.060	1.947
400	2.292	2.050	1.860
600	2.292	2.042	1.811
800	2.292	2.037	1.785
1000	2.292	2.033	1.770