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CROSS SECTION AND DEPLETION EQUATIONS FOR KARE AND FLAME

Compiled by
J. M. Shinn and D. E. Turcotte

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I Introduction

These are the specifications for the cross section and depletion calculations to be included in the few-group neutron diffusion codes KARE and FLAME. KARE is a two-dimensional code for the Philco Transac S-2000, being written at KAPL. FLAME is a three-dimensional code for the Remington-Rand LARC, being written at David Taylor Model Basin. FLAME will also include cross section and depletion calculations specified by Bettis Atomic Power Laboratory.

The formulations given here involve the work of many KAPL people; we will mention only R.W. Deutsch, who did the basic work.

The cross section calculation provides input for a 3-group neutron diffusion calculation which will normally be done immediately after the cross section calculation. The cross section calculation and the diffusion calculation provide input for a depletion calculation, which will normally be done immediately after the diffusion calculation. The regional power fractions computed by the diffusion code, and the new masses of fuel and poison computed by the depletion code, are in turn input for a later cross section calculation.

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Application of these specifications to FLAME.

In the first place, FLAME should allow for diffusion calculations in which the group constants for some material regions are provided as input by the user, and the constants for other regions are calculated by the cross section code specified here. Moreover, the possibility that all constants will be provided by one of these means and none by the other should be allowed for.

In the second place, FLAME should allow for life studies.

A life study consists first of a main sequence of problems, all run with steady-state xenon, by which the fuel and poison loadings in the material regions are computed as functions of time, and the steady-state power distribution is computed at each time for which fuel and poison loadings are obtained. In most cases each problem in the sequence is required to be critical, so that the control rod positions in each problem must have been found by a criticality search. For each problem in the sequence, fuel and poison loadings will be the output of the previous problem in the sequence, and the power in each region in the cross section input will be the product of the fractional power in the region computed in the diffusion calculation of the previous problem of the sequence, and reactor normal operating power, and input quantity.

In addition, a life study may contain peak xenon and no xenon problems, done at various times in the reactor life-time. These may be done between problems of the main sequence, or may be done after the main sequence is finished. They may involve criticality search. For each one, the fuel and poison loadings and the powers for the material regions must be obtained from the results of problems in the main sequence. Note that the power distribution at a given time is output from the main sequence problem for that time, whereas the fuel and poison distribution at that time are output of the previous main sequence problem. Peak xenon and no xenon problems will not include depletion calculations.

Two means of representing control rods are used.

Control rods may be represented explicitly. In this case the presence of control rods in a region of the reactor is represented byusing one material index for that region, and the absence of rods is indicated by using another index. Both materials will be non-fuel materials, for which depletion calculations are not done, and in which cross section input is not a function of reactor life-time.

Control rods may be represented by the "window-shade" method. In this case material index use remains constant; the presence of rods in the material region is indicated by the use of $\mathcal{Y}$-factors, and the absence of rods is indicated by not using these factors. The materials in which $\mathcal{Y}$-factors are used will be fuel regions, subject to depletion.

II Cross Sections

A. Input

General Input

A temperature and moderator density must be supplied for the reactor.

A power fraction should be supplied if a peak xenon condition is desired for a fractional power of the reactor steady-state operating power.

If it is desired to include the effect of resonance absorption of fission fragments in the epithermal group, an option for this should be included in the general input.

Cross sections may be all calculated from region-wise input; they may be all pre-calculated (as for example a four-group problem); or they may be partially machine calculated and partially pre-calculated. This option must be included in the general input.

The number of groups in the problem should be specified in the general input. The cross section code can calculate cross sections for three groups only. However, an output edit can be handled for up to five groups, and adjoint calculations can be done for four groups of pre-calculated input as well as for three group problems.

If an adjoint calculation is desired, either as an adjoint only or an adjoint and flux calculation, this should be so specified in the general input.

The following input is required in the general input for the calculation of $\mathcal{F}$ factors

$$\left.\begin{matrix} Q^2 \\ \\ \\ Q^3 \end{matrix}\right\} \frac{1}{\dfrac{2\ f\ \xi^g}{2-2\ f\ \xi^g}}$$

denominator is interpreted from Figure 1, SP-10.

2ℓ - (blade length)x2 in cm.

p - perimeter

A - area of fuel

Region-wise Input for Fuel Regions

Masses

$$\left.\begin{matrix} M^A_o \\ \\ M^A_t \\ \\ M^A_{t-1} \end{matrix}\right\} \text{Fuel}$$

$$\left.\begin{matrix} B^A_{h_o} \\ \\ B^A_{h_t} \\ \\ B^A_{h_{t-1}} \end{matrix}\right\} \text{Homogeneous poison}$$

$$\left.\begin{array}{l} B^{A}_{d_o} \\ \\ B^{A}_{d_t} \\ \\ B^{A}_{d_{t-1}} \end{array}\right\}\quad\text{Discrete poison}$$

B^M Non-burnable poison

All masses are actual masses for initial, present, and last time steps.

The present and initial time step values are used in the calculation of effective masses for no xenon, steady state xenon, or transient xenon conditions. The last and initial time step values are used in calculating the effective masses for peak xenon conditions.

Self-shielding parameters

Two sets of self-shielding parameters are required for any temperature. The first set is used if unrodded values are desired, and the second set if rodded values are desired.

Temperature

$$\left.\begin{array}{l} K_u^2 \\ K_u^3 \\ \gamma_u^2 \\ \gamma_u^3 \\ K_{pd}^2 \\ K_{pd}^3 \\ \gamma_{pd}^2 \\ \gamma_{pd}^3 \\ \gamma_{ph}^2 \\ \gamma_{ph}^3 \end{array}\right\} \text{Unrodded values}$$

$$\left.\begin{array}{l} K_u^2 \\ K_u^3 \\ \gamma_u^2 \\ \gamma_u^3 \end{array}\right\} \text{Rodded values}$$

$$\left.\begin{array}{l} K^{2}_{pd} \\ K^{3}_{pd} \\ \gamma^{2}_{pd} \\ \gamma^{3}_{pd} \\ \gamma^{2}_{ph} \\ \gamma^{3}_{ph} \\ g^{1} \\ g^{2} \end{array}\right\} \text{Rodded values (continued)}$$

If K^3_u (unrodded) = 0, it is assumed that the given masses are effective. In this case, all the poison must be homogeneous, otherwise a depletion cannot be done. The program will automatically set $f^2_u = f^3_u = 1$ if effective masses are supplied.

Input for Both Fuel and Non-fuel Regions

Volume of the region (in equations nomenclature is V_c)

Temperature option for the region

1. A general temperature for the reactor may be used.
2. A specific temperature may be given.
3. The effective temperature from a previously calculated region may be used.

(If the region contains fuel and an effective temperature is to be used, the self-shielding parameters will be used which correspond to the general temperature of the reactor.)

If either a general temperature or a specific temperature is desired, the code expects these values to be in degrees F.

Temperature or region number for desired effective temperature

If a specific temperature is desired for any region, the value must be given as a region dependent input.

If an effective temperature from a neighboring region is desired, the region number must be a region dependent input.

Moderator density option for the region

1. A general density for the reactor may be used
2. A specific density may be given
   (The moderator density used should correspond to the temperature used. Therefore, either the first or third temperature option would imply the general density, whereas if the specific temperature option is to be used, a specific moderator density should also be used.)

Specific moderator density as a region dependent input

Age option

The ages (τ^1 and τ^2) may be calculated by one of three sets of equations or supplied as region dependent input.

If specific ages are given, both τ^1 and τ^2 must be supplied. There are corresponding equations for τ^1 and τ^2, thus there is one option only for determing the method of calculating τ^1 and τ^2.

Ages, if supplied. Region dependent input

Xenon option

There are four possible xenon conditions for fuel regions. In non-fuel regions there can be no xenon. Fuel regions may have no xenon, or a xenon absorption contribution for steady-state, peak, or transient xenon conditions.

If either a steady-state or peak xenon calculation is desired, the power in megawatts must be supplied for the region. Further for a peak xenon calculation the power fraction of steady-state operating power may be supplied as a general input, that is as one value for the reactor.

If a transient xenon calculation is desired, the concentration of xenon atoms must be supplied.

Power in megawatts or xenon concentration

If a steady-state or peak xenon condition has been specified, the power must be supplied as a region dependent input.

If a transient xenon condition has been specified, the number of xenon atoms ($x10^{-18}$) must be supplied as a region dependent input.

Thin Region option

If thin region modifications to cross sections are desired, a thickness for the region must be supplied. If resonant absorbers are used, a P^2 should also be given as a region dependent input.

$\mathcal{H}$ - factor and self-shielding options

If unrodded self-shielding parameters are used,
there can be no $\mathcal{H}$-factors applied.

If rodded self-shielding parameters are used,
$\mathcal{H}$ — factors may be applied as follows:

- $\mathcal{H}$ – factors calculated
  - A's over $\mathcal{H}$'s
  - E's times $\mathcal{H}$'s
- $\mathcal{H}$ – factors supplied
  - A's over $\mathcal{H}$'s
  - E's times $\mathcal{H}$'s
- Skip $\mathcal{H}$-factor application

Effective masses supplied, $\mathcal{H}$ factors applied as follows:

- $\mathcal{H}$ - factors calculated
  - A's over $\mathcal{H}$'s
  - E's times $\mathcal{H}$'s
- $\mathcal{H}$ - factors supplied
  - A's over $\mathcal{H}$'s
  - E's times $\mathcal{H}$'s
- Skip $\mathcal{H}$- factor application

Perpendicular bucklings

Nine bucklings must be supplied per region, three for each group. The code will use only one of these per calculation. For each group, the following must be given $(B_m^g)^2$, $(B^g)^2$, $(B_M^g)^2$ where the subscripts signify as follows

m - minimum buckling guess
  - initial buckling guess, and the buckling to be used during calculation
M - maximum buckling guess

Coefficients for $\mathcal{F}$-factor variance with fuel depletion

If $\mathcal{F}$-factors are to be automatically varied with fuel depletion, four additional region-wise input quantities are required.

These quantities are b^2, b^3, c^2 and c^3.

Structural composition

The structural elements within each region must be specified. A sentinel is defined to signify a specific element. Each sentinel is distinct and should be followed by a volume (in equation nomenclature V_e) which designates the volume fraction which the specific element occupies.

B. Nomenclature

The nomenclature $x(T)$ will be used to specify that a temperature dependency exists for the variable, x. All temperatures referred to will be degrees Rankin unless otherwise specified.

For all variables which may be computed in more than one method, dependent upon options, both equations will be shown in the writeup, and the choice will be described in the region-wise input description.

The nomenclature $(B^g)^2$ is used to denote perpendicular buckling.

Group variables will be specified with superscripts. If powers are involved, the variable will be enclosed in parentheses.

The conversion from °Rankin to electronvolts is as follows e.v. = $^{\circ}R \times (0.47872 \times 10^{-4})$.

C. Equations

Fuel and poison concentration calculations

$$U_t = \frac{M_t^A}{M_o^A} \; ; \quad \text{for Peak Xenon} \quad U_t = \frac{M_{t-1}^A}{M_o^A}$$

$$P_{d_t} = \frac{B_{d_t}^A}{B_{d_o}^A} \; ; \quad \text{for Peak Xenon} \quad P_{d_t} = \frac{B_{d_{t-1}}^A}{B_{d_o}^A}$$

$$P_{h_t} = \frac{B_{h_t}^A}{B_{h_o}^A} \; ; \quad \text{for Peak Xenon} \quad P_{h_t} = \frac{B_{h_{t-1}}^A}{B_{h_o}^A}$$

Thermal self-shielding factors

$$f_u^3 = f_{p_h}^3 = \frac{K_u^3}{1 + \gamma_u^3 U_t + \gamma_{p_h}^3 P_{h_t}}$$

$$f_{p_d}^3 = \frac{K_{p_d}^3}{1 + \gamma_{p_d}^3 P_{d_t}}$$

Thermal effective masses

$$M^E_{t3} = M^A_o U_t f^3_u$$

$$B^E_{t3} = B^A_{d_o} P_{d_t} f^3_{p_d} + B^A_{h_o} P_{h_t} f^3_{p_h} + M^A_o f(1-U_t) f^3_{p_h} + B^M$$

or

$$= B^A_{d_o} P_{d_t} f^3_{p_d} + B^A_{h_o} P_{h_t} f^3_{p_h} + M^A_o f_1(1-U_t) f^3_{p_h} + B^M$$

The values of $f(1-U_t)$, $f_1(1-U_t)$, or $f_2(1-U_t)$ are linearly interpolated from the following tables.

$(1-U_t)$	$f(1-U_t)$
0.0	0
0.010	6.560×10^{-5}
0.025	9.700×10^{-5}
0.050	1.206×10^{-4}
0.125	1.534×10^{-4}
0.260	1.967×10^{-4}
0.470	2.544×10^{-4}
0.680	3.016×10^{-4}
0.760	3.147×10^{-4}
0.835	3.189×10^{-4}
1.000	3.168×10^{-4}

The following values are used to include the effect of resonance absorption of fission fragments in the epithermal group

$(1-U_t)$	$f_1(1-U_t)$	$f_2(1-U_t)$
0.01	0.41175×10^{-4}	1.73
0.05	0.10440×10^{-3}	2.44
0.10	0.13190×10^{-3}	2.94
0.20	0.16820×10^{-3}	3.81
0.30	0.19860×10^{-3}	4.36
0.40	0.22680×10^{-3}	4.73
0.50	0.25280×10^{-3}	4.97
0.60	0.27610×10^{-3}	5.14
0.70	0.29540×10^{-3}	5.32
0.80	0.30780×10^{-3}	5.39
1.00	0.0	0.0
0.85	0.31140×10^{-3}	5.51
0.90	0.30850×10^{-3}	5.72
0.95	0.29710×10^{-3}	6.23
1.00	0.2748×10^{-3}	6.93

[redacted]ermal self-shielding factors

$$f_u^2 = f_{p_h}^2 = \frac{K_u^2}{1 + \gamma_u^2 U_t + \gamma_{p_h}^2 P_{h_t}}$$

$$f_{p_d}^2 = \frac{K_{p_d}^2}{1 + \gamma_{p_d}^2 P_{d_t}}$$

Epithermal effective poison masses

$$B^E_{t_2} = B^A_{d_o} P_{d_t} f^2_{p_d} + B^A_{h_o} P_{h_t} f^2_{p_h} + M^A_o \mathit{f}(1-U_t) f^2_{p_h} + B^M$$

or

$$= B^A_{d_o} P_{d_t} f^2_{p_d} + B^A_{h_o} P_{h_t} f^2_{p_h} + \mathit{f}_2(1-U_t) M^A_o \mathit{f}_1(1-U_t) f^2_{p_h} + B^M$$

Pre-calculations, before actual cross sections are computed:

γ is dependent upon the type of xenon, and will be described under the xenon option.

$$\sigma_{a_u} = 0.27769/\sqrt{T \text{ ev}}$$

$$\xi \sum_s = \xi \sigma_{s_{H_2O}} (\rho V_{H_2O}) + \sum_e \xi \sigma_{s_e} V_e$$

$$\sum^3_{a_T} = \frac{\overline{M}^E_{t3}}{V_c} \sigma_{a_u} + \frac{B^E_{t3}}{V_c} \sigma^3_{a_B}(T) + \rho V_{H_2O} \sigma^3_{a_{H_2O}}(T)$$

$$+ \sum_e \sigma^3_{a_e}(T) V_e + \gamma \frac{P}{V_c}$$

Effective temperature

$$T_{eff} = T\left[1 + \frac{0.75\sum^{3} a_T}{\xi \bar{\Sigma}_s}\right]^2$$

There is an option available whereby the effective temperature from a region of lower index may be used as the effective temperature for the region.

Thermal cutoff

$$u_c = 24.68 - \ln T_{eff}$$

$$K_a = \frac{1}{0.93(u_c - 4.0)}$$

$$K_f = 0.877\, K_a$$

Age factors

$$\tau^1 = \frac{24.0}{(\rho\, V_{H_2O} + \sum_e e_e V_e)(\rho\, V_{H_2O} + \sum_e f_e V_e)}$$

or

$$= \frac{21.0}{(\rho V_{H_2O} + \sum_e e_e V_e)(\rho V_{H_2O} + \sum_e f_e V_e)}$$

or

$$= \frac{20.3}{(\rho V_{H_2O} + \sum_e e_e V_e)(\rho V_{H_2O} + \sum_e f_e V_e)}$$

$$\tau^2 = \frac{0.44\, u_c}{(\rho V_{H_2O} + \sum_e g_e V_e)(\rho V_{H_2O} + \sum_e h_e V_e)}$$

or

$$= \frac{0.44 u_c - 0.43}{(\rho V_{H_2O} + \sum_e g_e V_e)(\rho V_{H_2O} + \sum_e h_e V_e)}$$

or

$$= \frac{0.44\, u_c - 0.74}{(\rho V_{H_2O} + \sum_e g_e V_e)(\rho V_{H_2O} + \sum_e h_e V_e)}$$

Thermal group cross sections

$$\sigma_u^3 = \frac{108.6 - 410.4\ T_{eff}\ \text{e.v.} + 2926\ (T_{eff}\ \text{e.v.})^2}{\sqrt{T_{eff}\ \text{e.v.}}}$$

$$\sum a_u^3 = \frac{2.5617\ (10^{-3})\ M_{t3}^E\ \sigma_u^3}{V_c}$$

$$\sigma_p^3 = \frac{606.5}{\sqrt{T_{eff}\ \text{e.v.}}}$$

$$\sum a_B^3 = \frac{0.93\ B_{t3}^E\ \sigma a_B^3\ (T_{eff})}{V_c}$$

$$\sum a_e^3 = 0.93 \left[\rho\ V_{H_2O}\ \sigma a_{H_2O}^3\ (T_{eff}) + \sum_e V_e\ \sigma_{a_e}^3\ (T_{eff}) \right]$$

$$\sum a^3 = \sum a_u^3 + \sum a_B^3 + \sum a_e^3 + \sum a_{xe}^3$$

$$A^3 = \sum a^3 + D^3\ (B^3)^2$$

$$F^3 = \frac{\sum a_u^3}{1.184}$$

$$\bar{\Sigma}^{3}_{tr} = \bar{\Sigma}^{3}_{a} - \bar{\Sigma}^{3}_{axe} + \frac{\gamma P}{V_c} + \sum_{e} \sigma^{3}_{tr_e} V_e + \rho V_{H_2O} \sigma_{tr_{H_2O}} (T_{eff})$$

$$+ V_{CH_2} \sigma^{3}_{tr_{CH_2}} (T_{eff})$$

$$D^3 = \frac{1}{3 \bar{\Sigma}^{3}_{tr}}$$

$$Z^3 = \sqrt{A^3 D^3}$$

Epithermal group cross sections

$$\bar{\Sigma}^{2}_{tr} = \rho V_{H_2O} \sigma^{2}_{tr_{H_2O}} + \sum_{e} \sigma^{2}_{tr_e} V_e$$

$$D^2 = \frac{1}{3 \bar{\Sigma}^{2}_{tr}}$$

$$E^2 = \frac{D^2}{\tau^2}$$

$$\Delta \overline{\sum} a^2 = 0.0$$

or

$$= (V_{SAR\ Zirconium} + V_{SAR\ Zircaloy})\ 0.00425$$

or

$$= (V_{D1G\ Zirconium} + V_{D1G\ Zircaloy}) \left[0.0034 - \frac{0.206}{(u_c - 4.0)\sqrt{T_{eff}}} \right]$$

$$\overline{\sum} a^2 = K_a \left(\frac{f_u^2}{f_u^3} \overline{\sum} a_u^3 + \frac{B_{t2}^E}{B_{t3}^E} \overline{\sum} a_B^3 + \sum a_e^3 \right) + \Delta \overline{\sum} a^2$$

$$A^2 = \overline{\sum} a^2 + E^2 + D^2 (B^2)^2$$

$$F^2 = F^3 K_f \frac{f_u^2}{f_u^3}$$

$$Z^2 = \sqrt{A^2\ D^2}$$

$$\sigma_u^2 = K_a\ \sigma_u^3$$

$$\sigma_p^2 = K_a\ \sigma_p^3$$

Fast group cross sections

$$\Sigma^{1}_{tr} = \rho V_{H_2O} \sigma^{1}_{tr_{H_2O}} + \sum_{e} \sigma^{1}_{tr_e} V_e$$

$$D^{1} = \frac{1}{3 \Sigma^{1}_{tr}}$$

$$E^{1} = \frac{D^{1}}{\tau^{1}}$$

$$\Sigma^{1}_{a} = 0.0$$

$$A^{1} = \Sigma^{1}_{a} + E^{1} + D^{1}(B^{1})^{2}$$

$$Z^{1} = \sqrt{A^{1} D^{1}}$$

Xenon conditions

No xenon

$\gamma = 0.0$

$\overline{\sum} a_{xe}^3 = 0.0$

Steady state, peak, transient xenon

$$\bar{\sigma}_{xe}^3 = \frac{0.6994 - 4.38 \ (T_{eff} \text{ e.v.}) + 17.5 \ (T_{eff} \text{ e.v.})^2 \text{ mega-barns}}{\sqrt{T_{eff} \text{ e.v.}}}$$

$$\bar{F} = \frac{1}{1 + \dfrac{F^2 \ (\overline{\sum} a^3 - \overline{\sum} a_{xe}^3)}{F^3 \ E^2}}$$

Steady state and peak xenon

$$\phi^3 = \frac{0.003125 \ P \ \bar{F}}{F^3 \ V_c}$$

Steady state xenon

$\gamma = 0.0$

$$\bar{\sum} a^3_{xe_{ss}} = \frac{.002\ P\ \bar{\sigma}_{xe}}{V_c\ (0.2092 \times 10^{-4} + \phi^3 \bar{\sigma}^3_{xe})}$$

Peak xenon

$\gamma = f$(power fraction of steady state power) for p.f. = 1.0, $\gamma = 20.0$; for p.f. = 0.0, $\gamma = 72.9$

For intermediary values, a linear interpolation is performed to compute γ.

In the following equation f will be used to denote power fraction.

$\lambda_{xe} = 2.092 \times 10^{-5}\ \sec^{-1}$

$\lambda_{io} = 2.874 \times 10^{-5}\ \sec^{-1}$

$$B = \frac{\lambda_{xe}}{\lambda_{xe} + \bar{\sigma}^3_{xe}\,\phi^3} \left\{ \frac{f(\lambda_{xe} + \bar{\sigma}^3_{xe}\,\phi^3)}{\lambda_{xe} + f\,\bar{\sigma}^3_{xe}\,\phi^3} + \left[1 - \frac{f(\lambda_{xe} + \bar{\sigma}^3_{xe}\,\phi^3)}{\lambda_{xe} + f\,\bar{\sigma}^3_{xe}\,\phi^3} \right. \right.$$

$$\left. - \frac{(\lambda_{xe} + \bar{\sigma}^3_{xe}\,\phi^3)(1-f)}{\lambda_{xe} + f\,\bar{\sigma}^3_{xe}\,\phi^3 - \lambda_{io}} \right] \left[\frac{\lambda_{xe}(\lambda_{io} + \bar{\sigma}^3_{xe}\,\phi^3) + f(\bar{\sigma}^3_{xe}\,\phi^3)^2}{\lambda_{io}(\lambda_{xe} + \bar{\sigma}^3_{xe}\,\phi^3)} \right]^{\frac{\lambda_{xe} + f\bar{\sigma}^3_{xe}\,\phi^3}{\lambda_{io} - \lambda_{xe} - f\bar{\sigma}^3_{xe}\,\phi^3}}$$

$$+ \frac{(\lambda_{xe}+\bar{\sigma}^{3}_{xe}\, \phi^{3})(1-f)}{\lambda_{xe}+f\bar{\sigma}^{3}_{xe}\, \phi^{3}-\lambda_{io}} \left[\frac{\lambda_{xe}(\lambda_{io}+\bar{\sigma}^{3}_{xe}\, \phi^{3})+f(\bar{\sigma}^{3}_{xe}\phi^{3})^{2}}{\lambda_{io}(\lambda_{xe}+\bar{\sigma}^{3}_{xe}\phi^{3})} \right]^{\frac{\lambda_{io}}{\lambda_{io}-\lambda_{xe}-f\bar{\sigma}^{3}_{xe}\, \phi^{3}}} \Bigg\}$$

$$\sum a^{3}_{xe_{pk}} = \frac{95.6\ P\ \bar{\sigma}_{xe}\ B}{V_{c}}$$

Transient xenon

$$\gamma = 1.8$$

$$\sum a^{3}_{xe_{transient}} = \bar{\sigma}^{3}_{xe}\ \frac{(\text{Number xenon atoms} \times 10^{-18})}{V_{c}}$$

Thin Region Calculations

These calculations modify the previously calculated cross sections. The modified values replace the original cross sectional values, and additional modifications are applied to the new "effective" cross sections.

Fast group

Cross sections are not modified by thin region calculations

Epithermal group

$$\xi^{2} = t\left(\frac{1}{3D^{2}} + \sum a^{2} + E^{2}\right)$$

$$f^2 = \begin{cases} \dfrac{1}{1.0+1.6\xi^2} & \xi^2 \leq 2.0 \\[2ex] \dfrac{1}{0.2+2.0\xi^2} & \xi^2 > 2.0 \end{cases}$$

$$p^2 = 1 - 3\,D^2 \left(\sum a^2 + E^2 \right)$$

$$\epsilon^2 = \frac{f^2}{1 - p^2(1-f^2)}$$

$$P^2 = 1.0 - \frac{1.25\,\ln\left[\dfrac{1 + 0.86t\,(\sum a^3)}{1 + 0.86t\,(\sum a^3) \qquad \left(\dfrac{4T_{\text{eff}}^{\text{e.v.}}}{180000} \right)^{1/2}} \right]}{\ln\left[\dfrac{180000}{4\,T_{\text{eff}}^{\text{e.v.}}} \right]^{1/2}}$$

There is an option available which permits a value of P^2 to be supplied, rather than calculated.

$$\sum a^2_{\text{eff}} = \frac{1-P^2}{t(1+P^2)}$$

$$\alpha^2 = \frac{\sum a^2_{eff}}{\sum a^2}$$

$$E^1_{eff} = \alpha^2 E^1$$

$$F^2_{eff} = \alpha^2 F^2$$

$$\beta^2 = \frac{1}{\xi^2 f^2} - \frac{\alpha^2}{\epsilon^2}$$

$$D^2_{eff} = 0.25 \, t \, \beta^2$$

$$A^2_{eff} = \sum a^2_{eff} + \alpha^2 E^2 + D^2_{eff} (B^2)^2$$

Thermal group

$$\xi^3 = \frac{t}{3D^3}$$

$$f^3 = \begin{cases} \dfrac{1}{1.0+1.6\xi^3} & \xi^3 \leq 2.0 \\ \dfrac{1}{0.2+2.0\xi^3} & \xi^3 > 2.0 \end{cases}$$

$$p^3 = 1 - 3 \left(\overline{\sum} a^3\right) D^3$$

$$\epsilon^3 = \frac{f^3}{1-p^3(1-f^3)}$$

$$\alpha^3 = \frac{\epsilon^3}{1-t\left(\overline{\sum} a^3\right)D^3}$$

$$\overline{\sum} a^3_{eff} = \alpha^3\left(\overline{\sum} a^3\right)$$

$$E^2_{eff} = \alpha^3 E^2 \alpha^2$$

$$F^3_{eff} = \alpha^3 F^3$$

$$\beta^3 = \frac{1}{\xi^3 f^3} - \frac{\alpha^3}{\epsilon^3}$$

$$D^3_{eff} = 0.25\ t\ \beta^3$$

$$A^3_{eff} = \sum a^3_{eff} + D^3_{eff}\ (B^3)^2$$

These calculations are reasonable only for $\frac{1}{v}$ absorbers which do not contain hydrogen. Resonant absorbers which do not have hydrogen mixed with them can be treated by inserting a P^2.

Rod representation - $\mathcal{J}$ factors

These values may be calculated or inserted.

Precalculations for $\mathcal{J}$ factors

$$d^2 = 2\ D^2\ Q^2$$

$$X_o = A/p$$

$$M = \sqrt{\frac{D^2}{E^2 + \sum a^2}}$$

$$M_{eff} = \frac{M \tanh \frac{X_o}{M}}{1 + \frac{d^2}{M} \tanh \frac{X_o}{M}}$$

$$\phi^2 = 1 + \frac{0.28}{2\ell} M_{eff}$$

$$d^3 = 2 D^3 Q^3$$

$$L = \sqrt{\frac{D^3}{\sum a^3}}$$

$$L_{eff} = \frac{L \tanh \frac{X_o}{L}}{1 + \frac{d^3}{L} \tanh \frac{X_o}{L}}$$

$$\phi^3 = 1 + \frac{0.28}{2\ell} L_{eff}$$

$\mathcal{J}$ - factors

$$\mathcal{J}^2 = 1 - M_{eff} \left(\frac{p \phi^2}{A} \right)$$

$$\mathcal{J}^3 = 1 - \frac{1}{\mathcal{J}^2} \left(L_{eff} \frac{p \phi^3}{A} \right) \left\{ 1 - \frac{\left[1 - \frac{L \tanh \frac{X_o}{M}}{M \tanh \frac{X_o}{L}} \right]}{\left(1 - \frac{L^2}{M^2}\right)\left(1 + \frac{d^2}{M} \tanh \frac{X_o}{M}\right)} \right\}$$

It is also possible to automatically vary $\mathcal{J}$-factors with fuel depletion according to the following formulae.

$$\mathcal{J}_t^2 = \mathcal{J}_o^2 \left[1 + (U_t - 1)\, b^2 + (U_t^2 - 1)\, c^2 \right]$$

$$\mathcal{J}_t^3 = \mathcal{J}_o^3 \left[1 + (U_t - 1)\, b^3 + (U_t^2 - 1)\, c^3 \right]$$

where $\mathcal{J}_t$ = $\mathcal{J}$-factor at time t

$\mathcal{J}_o$ = $\mathcal{J}$-factor at initial time

U_t = Fuel fraction remaining at time t

If $b^2 = b^3 = c^2 = c^3 = 0$, then $\mathcal{J}$-factors can be held constant throughout depletion.

$\mathcal{J}$-factor application

If $\mathcal{J}$-factors are applied, the previously calculated cross sections are modified, and the modified values replace the previous cross sections so that any additional modifications are made to these new "effective" cross sections.

$\mathcal{J}$-factors inversely applied to A's

$$A_{eff}^2 = \frac{A^2}{\mathcal{J}2}$$

$$A_{eff}^3 = \frac{A^3}{\mathcal{J}3}$$

$\mathcal{G}$ factors directly applied to E's

$$E^1_{eff} = E^1 \mathcal{G}^2$$

$$E^2_{eff} = E^2 \mathcal{G}^3$$

Adjoint calculations

Adjoints may be computed for either three or four group flux input.

Three Group Flux		Three Group Adjoint
D^1		D^3
A^1		A^3
F^1	In non-core region $\chi = F = 0$	χ^3
χ^1		F^3
Z^1		Z^3
D^2		D^2
E^1		E^2
A^2		A^2
F^2	In non-core region $\chi = F = 0$	χ^2
χ^2		F^2
Z^2		Z^2

D^3		D^1
E^2		E^1
A^3		A^1
F^3	In non-core region $\chi = F = 0$	χ^1
χ^3		F^1
Z^3		Z^1

Flux input must be pre-calculated

Four Group Flux		Four Group Adjoint
D^1		D^4
A^1		A^4
F^1	In non-core region $\chi = F = 0$	χ^4
χ^1		F^4
Z^1		Z^4
D^2		D^3
E^1		E^3
A^2		A^3
F^2	In non-core region $\chi = F = 0$	χ^3
χ^2		F^3
Z^2		Z^3

D^3
E^2
A^3
F^3 In non-core region $\chi = F = 0$
χ^3
Z^3

D^2
E^2
A^2
χ^2
F^2
Z^2

D^4
E^3
A^4
F^4 In non-core region $\chi = F = 0$
χ^4
Z^4

D^1
E^1
A^1
χ^1
F^1
Z^1

Nu timesF

$\nu = 2.46$

Calculate

$\nu F^2 = 2.46 F^2$

$\nu F^3 = 2.46 F^3$

Criticality coefficient - $K_{\text{effective}}$

$$K_{\text{eff}} = \frac{\nu E^1 (E^2 F^3 + F^2 A^3)}{A^1 A^2 A^3}$$

D. Output

Edited decimal output

Macroscopic Cross sections

D^1		Σ_a^1		$D^1(B^1)^2$	Z^1	A^1	K_{eff}
D^2	E^1	Σ_a^2	νF^2	$D^2(B^2)^2$	Z^2	A^2	
D^3	E^2	Σ_a^3	νF^3	$D^3(B^3)^2$	Z^3	A^3	

This output will be printed per region

Edited binary output

Macroscopic cross sections

$$\begin{array}{cccccc}
D_1^1 & & A_1^1 & & Z_1^1 & \gamma_1^1 \\
\vdots & & & & & \\
D_1^2 & E_1^1 & A_1^2 & F_1^2 & Z_1^2 & \gamma_1^2 \\
\vdots & & & & & \\
D_1^3 & E_1^2 & A_1^3 & F_1^3 & Z_1^3 & \gamma_1^3
\end{array}$$

This output will be written per group.

Microscopic absorption cross sections

$$\begin{array}{l}
\bar{\Sigma}\, a_1^1 \\
\vdots \\
\bar{\Sigma}\, a_1^2 \\
\vdots \\
\bar{\Sigma}\, a_1^3
\end{array}$$

This output will be written per group.

Depletion input

$$\begin{array}{ccccccccc}
M_o^A & B_{d_o}^A & B_{h_o}^A & M_t^A & B_{d_t}^A & B_{h_t}^A & U_t & P_{d_t} & P_{h_t} \\
\gamma_u^2 & \gamma_u^3 & \gamma_{pd}^2 & \gamma_{pd}^3 & \gamma_{ph}^2 & \gamma_{ph}^3 & K_u^2 & K_u^3 & K_{pd}^2 \\
K_{pd}^3 & \sigma_u^2 & \sigma_u^3 & \sigma_p^2 & \sigma_p^3 & & & &
\end{array}$$

This output will be written per region.

Library Microscopic Cross Sections and Age Equivalence Factors

Substance	$\sigma_a^3(T)$	$\xi\sigma_s$	Age Equivalence Factors				σ_{tr}^1	σ_{tr}^2	$\sigma_{tr}^3(T_{eff})$
			e	f	g	h			
Boron - 10	5270.0	-	-	-	-	-			
Water	0.5078	1.3540	0	0	0	0	0.2016	0.5496	$\frac{52.58}{\sqrt{T_{eff}}} + 0.1304$
Zirconium	0.1769	0.0074	0.109	1.33	0.005	0.547	0.2650	0.2993	0.2620
Aluminum	0.3194	0.0061	0.103	0.922	0.006	0.195	0.1859	0.1074	0.0845
Iron	4.9290	0.0330	0.186	1.20	0.021	1.390	0.2425	0.7573	0.9670
Stainless Steel	5.6640	0.0330	0.186	1.20	0.021	1.390	0.2425	0.7573	0.9670
Zircaloy	0.2060	0.0074	0.109	1.33	0.005	0.547	0.2650	0.2993	0.2620
C_2H_4	0.6055	1.6090	1.190	1.06	1.190	1.230	0.2137	0.6782	$\frac{62.13}{\sqrt{T_{eff}}} + 0.1778$
Inconel	8.7000	0.0440	0.209	1.53	0.034	2.300	0.3090	1.2600	1.2800
SAR Zirconium	0.1769	0.0074	0.109	1.33	0.005	0.547	0.2650	0.2993	0.2620
SAR Zircaloy	0.2060	0.0074	0.109	1.33	0.005	0.547	0.2650	0.2993	0.2620
D1G Zirconium	0.1769	0.0074	0.109	1.33	0.005	0.547	0.2650	0.2993	0.2620
D1G Zircaloy	0.2060	0.0074	0.109	1.33	0.005	0.547	0.2650	0.2993	0.2620

Other elements may be added

III Depletion

A. Input (region-wise)

Output from cross section calculations

a)	M_o^A	Original actual mass of fuel
b)	$B_{d_o}^A$	Original actual mass of boron discretely distributed
c)	$B_{h_o}^A$	Original actual mass of boron homogeneously distributed
d)	M_t^A	Actual mass of fuel at time step t
e)	$B_{d_t}^A$	Actual mass of discrete boron at time t
f)	$B_{h_t}^A$	Actual mass of homogeneous boron at time t
g)	U_t	Concentration of fuel at time t
h)	P_{d_t}	Concentration of discrete boron at time t
i)	P_{h_t}	Concentration of homogeneous boron at time t
j)	γ_u^2	self-shielding factors
k)	γ_u^3	
l)	$\gamma_{p_d}^2$	
m)	$\gamma_{p_d}^3$	

$$\left.\begin{array}{ll} \text{n)} & \gamma^{2}_{p_h} \\ \text{o)} & \gamma^{3}_{p_h} \\ \text{p)} & K^{2}_{u} \\ \text{q)} & K^{3}_{u} \\ \text{r)} & K^{2}_{p_d} \\ \text{s)} & K^{3}_{p_d} \end{array}\right\} \text{self-shielding factors (continued)}$$

$$\left.\begin{array}{ll} \text{t)} & \sigma^{2}_{u} \\ \text{u)} & \sigma^{3}_{u} \\ \text{v)} & \sigma^{3}_{p} \\ \text{w)} & \sigma^{3}_{p} \end{array}\right\} \text{microscopic absorption cross sections}$$

Other

a)	power fractions	$P\ell/P$
b)	volumes	Vol.
c)	flux integrals group 2	$\int \phi^2 dV$
d)	flux integrals group 3	$\int \phi^3 dV$
e)	total fuel depletion in the time step	ΔF

Item e is the only non-region-dependent input to the depletion calculation. The requestor must supply ΔF for each time step.

a), b), c), and d) are to be computed as by-products of the diffusion calculation, for the material region in question.

Equations

Fuel concentration after depletion

$$U_{t+1} = U_t - \frac{P\ell/P \cdot \Delta F}{M_o^A}$$

where U_{t+1} is fuel concentration at time step t+1.

Actual fuel mass

$$M_{t+1}^A = M_o^A \cdot U_{t+1}$$

Boron concentration

$$\frac{1}{au} \ \ell n \ \frac{U_{t+1}}{U_t} + \left(\frac{bu^2 + au^2 du - au\ bu\ cu}{au\ bu^2} \right) \ \ell n \ \frac{au + bu\ U_t}{(au + bu\ U_{t+1})}$$

$$+ \frac{du}{bu} (U_{t+1} - U_t) = \frac{\sigma_u^3}{\sigma_p^3} \left[\frac{1}{ap} \ \ell n \ \frac{P_{t+1}}{P_t} + \left(\frac{bp^2 + ap^2 dp - ap\ bp\ cp}{ap\ bp^2} \right) \cdot \right.$$

$$\left. \ell n \ \frac{(a_p + b_p\ P_t)}{(ap + bp\ P_{t+1})} + \frac{dp}{bp} \left(P_{t+1} - P_t \right) \right]$$

where $au = gu \cdot K_u^2 + K_u^3$ $\qquad$ $gu = \dfrac{\sigma_u{}^2}{\sigma_u{}^3} \cdot \dfrac{\int \emptyset^2 dV}{\int \emptyset^3 dV}$

$$bu = gu \cdot K_u^2 \cdot \gamma_u^3 + K_u^3 \cdot \gamma_u^2$$

$$cu = \gamma_u^2 + \gamma_u^3$$

$$du = \gamma_u^2 \cdot \gamma_u^3$$

and $$ap = gp \circ K_{p_d}^2 + K_{p_d}^3 \qquad gp = \frac{\sigma_p^2}{\sigma_p^3} \circ \frac{\int \phi^2 dV}{\int \phi^3 dV}$$

$$bp = gp \cdot K_{p_d}^2 \cdot \gamma_{p_d}^3 + K_{p_d}^3 \circ \gamma_{p_d}^2$$

$$cp = \gamma_{p_d}^2 + \gamma_{p_d}^3$$

$$dp = \gamma_{p_d}^2 \circ \gamma_{p_d}^3$$

This equation is solved for P_{t+1} by Newton's Method: The first approximation for the iteration is $P_{(1)} = \frac{P_t}{2^n}$, where n is the least integer such that $F\left(\frac{P_t}{\lambda^n}\right) \angle 0$, and $F(P_{(g)})$ denotes (R.H.S. of boron concentration equation, with $P_{t+1} = P_{(g)}$) minus L.H.S. Then the Newton's Method iteration is

$$P_{(g+1)} = P_{(g)} - \frac{F(P_{(g)})}{F'(P_{(g)})}$$

as usual.

The iteration is considered to have converged when

$$P_{(g)} - P_{(g+1)} < \frac{P_{(g+1)}}{30}$$

b) boron homogeneously distributed

$$P_{h_t} = U^{\beta}_{t+1}$$

$$\text{where } \beta = \frac{\sigma^3_u}{\sigma^3_p} \left(\frac{1 + gp}{1 + gu} \right)$$

c) boron discretely distributed in combination case

$$\frac{K^3_{p_d}}{K^3_u} \cdot \beta \left[\ell n \frac{U_{t+1}}{U_t} + \gamma^3_u \, (U_{t+1} - U_t) + \frac{\gamma^{\;3}_{p_h} (U^{\beta}_{t+1} - U^{\beta}_t)}{\beta} \right]$$

$$= \ell n \frac{P_{d_{t+1}}}{P_{d_t}} + \gamma^{\;3}_{p_d} \, (P_{d_{t+1}} - P_{d_t})$$

This equation is solved in the same manner as case a.

Actual boron mass

a) discrete boron mass

$$B^A_{d_{t+1}} = B^A_{d_o} \cdot P_{d_{t+1}}$$

b) homogeneous boron mass

$$B^A_{h_{t+1}} = B^A_{h_o} \cdot P_{h_{t+1}}$$

Summations over all regions

a) fuel mass

$$\sum_R M^A_{t+1}$$

b) discrete boron mass

$$\sum_R B^A_{d_{t+1}}$$

c) homogeneous boron mass

$$\sum_R B^A_{h_{t+1}}$$

Weighted averages

a) fuel concentration

$$\frac{\sum_R U_{t+1}}{\sum_R \text{Vol.}}$$

b) discrete boron concentration

$$\frac{\sum_R P_{d_{t+1}}}{\sum_R \text{Vol.}}$$

c) homogeneous boron concentration

$$\frac{\sum_R P_{h_{t+1}}}{\sum_R \text{Vol.}}$$

Output

Input for next time step

a) M^A_{t+1}

b) $B^A_{d_{t+1}}$

c) $B^A_{h_{t+1}}$

d) M^A_t

e) $B^A_{d_t}$

f) $B^A_{h_t}$

Printed output

a) ℓ - region number

$$\left.\begin{array}{l} \text{b)}\ U_{t+1} \\ \text{c)}\ P_{d_{t+1}} \\ \text{d)}\ P_{h_{t+1}} \\ \text{e)}\ M^{A}_{t+1} \\ \text{f)}\ B^{A}_{d_{t+1}} \\ \text{g)}\ B^{A}_{h_{t+1}} \end{array}\right\}\ \text{regionwise}$$

h) $\sum_R M^A_{t+1}$

i) $\sum_R B^A_{d_{t+1}}$

j) $\sum_R B^A_{d_{t+1}}$

k) $\dfrac{\sum_R U_{t+1}}{\sum_R \text{Vol.}}$

l) $\dfrac{\sum_R P_{d_{t+1}}}{\sum_R \text{Vol.}}$

m) $\dfrac{\sum_R P_{h_{t+1}}}{\sum_R \text{Vol.}}$