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SUBJECT: (U) Sensitivity of an (α,n) Neutron Source to Nuclear Data

I. Introduction

Favorite and Weidenbenner presented first-order sensitivities of the (α,n) neutron source rate density (both magnitude and energy spectrum) with respect to isotopic number densities and material mass densities.[1] Favorite presented second-order sensitivities.[2]

This report presents derivatives of the (α,n) neutron source rate density to the (α,n) cross section and stopping power data that are passed to and used in SOURCES4C. These derivatives can be used in a classical "sensitivity analysis/uncertainty quantification" procedure, or they may be useful in the type of uncertainty quantification that was done in Ref. 3.

As in Ref. 1, we use the mathematical descriptions of the (α,n) neutron source rate density and energy spectrum that are used by SOURCES4C and described in the SOURCES4C manual;[4] specifically, a material's α-particle stopping power is given by the Bragg-Kleeman relationship.[5] Also, this report addresses the (α,n) neutron source generated in a homogeneously mixed material. This report does not account for the sensitivity of the (α,n) neutron source strength or spectrum to the crystal form of the material.

This report describes how (α,n) cross sections and stopping powers are computed in SOURCES4C using the nuclear data that are passed in.

The next section of this report summarizes how SOURCES4C computes the (α,n) neutron source rate density and spectrum given the (α,n) cross sections and stopping powers. Section III describes how SOURCES4C computes (α,n) cross sections and derives the derivative of the (α,n) neutron source rate density with respect to basic (α,n) cross section data. Section IV describes how SOURCES4C computes stopping powers and derives the derivative of the (α,n) neutron source rate density with respect to basic stopping power data. Section V briefly describes the modifications that were made to SOURCES4C to compute and output the derivatives. Section VI presents results of a test problem. Section VII is a summary and conclusions. The input file for the test problem is listed in the appendix.

II. Computation of an (α,n) Source

This section describes how SOURCES4C computes the (α,n) source for a homogeneously mixed material. (There are other methods available.[6]) This section generally follows the SOURCES4C manual[4] and repeats (with small modifications) the presentation in Ref. 1.

The stopping cross section ε of a material for α particles of energy E is defined as

$$\varepsilon(E) = -\frac{1}{N}\frac{dE}{dx}, \tag{1}$$

where N is the total atom density of the material and x is the path length of the α particle through the material. The stopping cross section can be calculated using the Bragg-Kleeman relationship[5]

$$\varepsilon(E) \cong \frac{1}{N}\sum_{j=1}^{J} N_j \varepsilon_j(E), \tag{2}$$

where $\varepsilon_j(E)$ and N_j are the stopping power and atom density of isotope j, respectively, and

$$N = \sum_{j=1}^{J} N_j. \tag{3}$$

Stopping powers depend on the element, not the isotope, so all isotopes of an element have the same stopping power.

The probability of an α particle of energy E_α undergoing an (α,n) reaction with nuclide i before stopping can be represented by the function

$$P_i(E_\alpha) = \frac{N_i}{N}\int_0^{E_\alpha} \frac{\sigma_i(E)}{\varepsilon(E)} dE. \tag{4}$$

In SOURCES4C, Eq. (4) is approximated as

$$P_i(E_\alpha) = \frac{N_i}{N}\sum_{g=1}^{G_\alpha}\frac{1}{2}\left[\frac{\sigma_{i,g+1}}{\varepsilon_{g+1}} + \frac{\sigma_{i,g}}{\varepsilon_g}\right](E_{g+1} - E_g), \tag{5}$$

where G_α, the number of α-particle energy bins, is a user input. The number of quadrature points in the numerical integral is, of course, $G_\alpha + 1$. For each α-emitting isotope in the material, the α-particle energy range is the largest discrete α-particle energy emitted, $E_{G_\alpha+1}$, minus the minimum allowable α-particle energy, either 0.001 MeV or the target's (α,n) threshold, whichever is larger. This range is divided by G_α to determine the α-particle energy group structure. Therefore, $E_{g+1} - E_g$ is the same for each energy bin and Eq. (5) is a simple trapezoid rule. For energies smaller than $E_{G_\alpha+1}$ (for each α-emitting isotope), the code computes P_i by interpolating on the group structure:

$$P_i(E_l) = P_i(E_{g_\alpha,l}) + \frac{E_l - E_{g_\alpha,l}}{E_{g_\alpha+1,l} - E_{g_\alpha,l}}\left[P_i(E_{g_\alpha+1,l}) - P_i(E_{g_\alpha,l})\right], \tag{6}$$

where $E_{g_\alpha,l}$ and $E_{g_\alpha+1,l}$ are the energy bins immediately below and above E_l, respectively ($E_{g_\alpha,l} \le E_l \le E_{g_\alpha+1,l}$). From Eq. (5), the value $P_i(E_{b_\alpha+1})$ at an energy $E_{b_\alpha+1}$ coinciding with a bin in the energy structure is

$$P_i(E_{b_\alpha+1}) = \frac{N_i}{N}\left\{\frac{1}{2}\left[\frac{\sigma_{i,1}}{\varepsilon_1}(E_2-E_1)+\frac{\sigma_{i,b_\alpha+1}}{\varepsilon_{b_\alpha+1}}(E_{b_\alpha+1}-E_{b_\alpha})\right]+\frac{1}{2}\sum_{g=2}^{b_\alpha-1}\frac{\sigma_{i,g}}{\varepsilon_g}(E_{g+1}-E_{g-1})\right\}$$
$$= \frac{N_i}{N}\left\{\frac{1}{2}\left[\frac{\sigma_{i,1}}{\varepsilon_1}+\frac{\sigma_{i,b_\alpha+1}}{\varepsilon_{b_\alpha+1}}\right]+\sum_{g=2}^{b_\alpha-1}\frac{\sigma_{i,g}}{\varepsilon_g}\right\}\left(\frac{E_{G_\alpha+1}-E_1}{G_\alpha}\right). \tag{7}$$

Note that the notation has changed slightly from that of Eq. (5): The index on the energy that is the argument of P_i is now the same as the index of the upper energy used in the sum (not the upper limit of the sum).

The multigroup form of Eq. (2) is used:

$$\varepsilon_g = \frac{1}{N}\sum_{j=1}^{J} N_j \varepsilon_{j,g}. \tag{8}$$

In Eqs. (5) through (8), g indexes the α-particle energy discretization used to evaluate Eq. (4).

The fraction of decays of nuclide k resulting in an (α,n) reaction in isotope i is

$$R_{k,i}(\alpha,n) = \sum_{l=1}^{L} f_{kl}^{\alpha} P_i(E_l), \tag{9}$$

where f_{kl}^{α} is the fraction of all decays of nuclide k resulting in an α particle of energy E_l and L is the number of discrete α particle energies emitted by nuclide k. The quantities L, f_{kl}^{α}, and E_l (l = 1,…,L) are given in the nuclear data for each α particle emitter (source isotope) k (specifically, these are given in SOURCES4C's `tape5` data file[4]).

The total neutron source rate density due to target i and α source k is

$$Q_{(\alpha,n),k,i} = \lambda_k N_k R_{k,i}(\alpha,n)$$
$$= \lambda_k N_k \sum_{l=1}^{L} f_{kl}^{\alpha} P_i(E_l), \tag{10}$$

where λ_k is the decay constant for nuclide k. Using Eq. (6), Eq. (10) becomes

$$Q_{(\alpha,n),k,i} = \lambda_k N_k \sum_{l=1}^{L} f_{kl}^{\alpha}\left\{P_i(E_{g_\alpha,l})+\frac{E_l-E_{g_\alpha,l}}{E_{g_\alpha+1,l}-E_{g_\alpha,l}}\left[P_i(E_{g_\alpha+1,l})-P_i(E_{g_\alpha,l})\right]\right\}. \tag{11}$$

Note that P_i contains the density of every nuclide [see Eqs. (5), (3), and (2)].

The total (α,n) neutron source rate density is the sum of $Q_{(\alpha,n),k,i}$ over all targets and sources:

$$Q_{(\alpha,n)} = \sum_k \sum_i Q_{(\alpha,n),k,i}. \tag{12}$$

We now turn to the calculation of the (α,n) neutron energy spectrum. This section differs slightly from the discussion in Ref. 4 (but it continues to repeat Ref. 1). The fraction of α particles from source isotope k reacting with target nuclide i resulting in product level m reactions occurring in α-particle energy group g is

$$F_{k,i,g}(m) = S_{i,g}(m) H_{i,g,l}, \tag{13}$$

where $H_{i,g,l}$ is the fraction of target *i* reactions of α particles of emission energy *l* in α-particle energy group *g*, equal to[a]

$$H_{i,g,l} = \frac{P_i(E_{g+1}) - P_i(E_g)}{P_i(E_l)}, \tag{14}$$

and $S_{i,g}(m)$ is the branching fraction to product level *m* of α particles of energy E_g, calculated using the interpolation

$$\begin{aligned} S_{i,g}(m) &= f_i(m,m'-1) + \left(f_i(m,m') - f_i(m,m'-1)\right) \\ &\times \frac{E_g - E(m'-1)}{E(m') - E(m'-1)}, \end{aligned} \tag{15}$$

where $f_i(m,m')$ is the fraction of (α,n) reactions with target *i* at energy $E(m')$ resulting in the production of product level *m*. The energy levels and fractions used in Eq. (15) are nuclear data for each target nuclide and do not depend on densities. [When the code computes Eq. (15) for each of the α-particle energies in the G_α-group structure, E_g is actually the midpoint each energy group rather than the endpoint.]

The (α,n) neutron energy spectrum $\chi_{k,i}^{(\alpha,n)}(E^g)$ is[b]

$$\begin{aligned} \chi_{k,i}^{(\alpha,n)}(E^g) &= R_{k,i}(\alpha,n) \\ &\times \sum_{l=1}^{L}\sum_{m=1}^{M}\sum_{g_\alpha=1}^{G_\alpha} F_{k,i,g_\alpha}(m) \frac{E^{g+1} - E^g}{E_{n,m}^{+}(E_{g_\alpha}) - E_{n,m}^{-}(E_{g_\alpha})}, \end{aligned} \tag{16}$$

where $E_{n,m}^{-}(E_{g_\alpha})$ and $E_{n,m}^{+}(E_{g_\alpha})$ are the minimum and maximum permissible neutron kinetic energies from an incident α particle of energy E_{g_α} that generates a product nuclide with level *m*, *M* is the number of product levels for target *k*, and the neutron group boundaries E^{g+1} and E^g are between $E_{n,m}^{-}(E_{g_\alpha})$ and $E_{n,m}^{+}(E_{g_\alpha})$. It is assumed that the neutrons are isotropically emitted and contribute uniformly to all groups between $E_{n,m}^{-}(E_{g_\alpha})$ and $E_{n,m}^{+}(E_{g_\alpha})$. Define

$$\Delta E_{m,g_\alpha}^{g} \equiv \frac{E^{g+1} - E^g}{E_{n,m}^{+}(E_{g_\alpha}) - E_{n,m}^{-}(E_{g_\alpha})}. \tag{17}$$

The total neutron source rate density in energy group *g* due to α emitter *k* and target *i* is

$$\begin{aligned} Q_{(\alpha,n),k,i}^{g} &= \lambda_k N_k \chi_{k,i}^{(\alpha,n)}(E^g) \\ &= Q_{(\alpha,n),k,i} \sum_{l=1}^{L}\sum_{m=1}^{M}\sum_{g_\alpha=1}^{G_\alpha} F_{k,i,g_\alpha}(m) \Delta E_{m,g_\alpha}^{g} \end{aligned} \tag{18}$$

[using Eq. (10)]. In Eqs. (16), (17), and (18), *g* indexes neutron energy groups and g_α indexes α energy groups.

The total neutron source rate density in energy group *g* due to α emitter *k* is the sum of $Q_{(\alpha,n),k,i}^{g}$ over targets; the total neutron source rate density in energy group *g* due to target *i* is the sum of $Q_{(\alpha,n),k,i}^{g}$ over

[a] Equation (32) in Ref. 4 indicates that *H* is a function of the product level *m*, but in the code, *H* is calculated for each of the $G_\alpha + 1$ energy bin boundaries in the group structure and does not depend on the product level.
[b] Equation (35) in Ref. 4 lacks the sums over discrete α energies *l*, product levels *m*, and α energy groups g_α.

α emitters. The total (α,n) neutron source rate density in energy group *g*, $Q^{g}_{(\alpha,n)}$, is the sum of $Q^{g}_{(\alpha,n),k,i}$ over α emitters and targets. The total (α,n) neutron source rate density $Q_{(\alpha,n)}$ is the sum of $Q^{g}_{(\alpha,n)}$ over neutron energy groups.

III. Derivative of the (α,n) Source Rate Density with Respect to the (α,n) Cross Section

From Eq. (10), the derivative of $Q_{(\alpha,n),k,i}$ with respect to the (α,n) cross section σ_{j,g_α} of isotope *j* in α energy group g_α is

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial \sigma_{j,g_\alpha}} = \lambda_k N_k \sum_{l=1}^{L} f^{\alpha}_{kl} \frac{\partial P_i(E_l)}{\partial \sigma_{j,g_\alpha}}. \tag{19}$$

Accounting for the interpolation at α emission energies below $E_{G_\alpha+1}$, i.e. using Eq. (11), the derivative is

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial \sigma_{j,g_\alpha}} = \lambda_k N_k \sum_{l=1}^{L} f^{\alpha}_{kl} \left\{ \frac{\partial P_i(E_{g_\alpha,l})}{\partial \sigma_{j,g_\alpha}} + \frac{E_l - E_{g_\alpha,l}}{E_{g_\alpha+1,l} - E_{g_\alpha,l}} \left[\frac{\partial P_i(E_{g_\alpha+1,l})}{\partial \sigma_{j,g_\alpha}} - \frac{\partial P_i(E_{g_\alpha,l})}{\partial \sigma_{j,g_\alpha}} \right] \right\}. \tag{20}$$

Energy E_{g_α} is an arbitrary point on the energy grid and energies $E_{g_\alpha,l}$ and $E_{g_\alpha+1,l}$ are still the energy bins immediately below and above an α emission energy E_l, respectively. Using Eq. (7), the derivative of $P_i(E_{g_\alpha,l})$ with respect to σ_{j,g_α} is

$$\frac{\partial P_i(E_{g_\alpha,l})}{\partial \sigma_{j,g_\alpha}} = \begin{cases} \delta_{ij} \dfrac{N_i}{N} \dfrac{1}{\varepsilon_{g_\alpha}} \left(\dfrac{E_{G_\alpha+1} - E_1}{G_\alpha} \right), E_{g_\alpha} < E_{g_\alpha,l} \\ \delta_{ij} \dfrac{N_i}{N} \dfrac{1}{2\varepsilon_{g_\alpha}} \left(\dfrac{E_{G_\alpha+1} - E_1}{G_\alpha} \right), E_{g_\alpha} = E_{g_\alpha,l} \\ 0, E_{g_\alpha} > E_{g_\alpha,l}, \end{cases} \tag{21}$$

where δ_{ij} is the Kronecker delta. A similar equation obtains for the derivative of $P_i(E_{g_\alpha+1,l})$.

The sum over the α emission energy index *l* in Eq. (20) should be broken into four components: $E_{g_\alpha} < E_{g_\alpha,l}$, $E_{g_\alpha} = E_{g_\alpha,l}$, $E_{g_\alpha} = E_{g_\alpha+1,l}$, and $E_{g_\alpha} > E_{g_\alpha+1,l}$. The fourth component is zero. See Figure 1. For $E_{l=1}$, for example, $E_{g_\alpha,l} = E_{g_\alpha=3}$ and $E_{g_\alpha+1,l} = E_{g_\alpha=4}$, while for $E_{l=2}$, $E_{g_\alpha,l} = E_{g_\alpha=4}$ and $E_{g_\alpha+1,l} = E_{g_\alpha=5}$. All cross sections at grid energies equal to or below an α emission energy contribute to $Q_{(\alpha,n),k,i}$ for that α emission energy; cross sections at grid energies above do not, except for the grid energy immediately above. (As in SOURCES4C, in Figure 1 the maximum grid energy is equal to the highest α emission energy.)

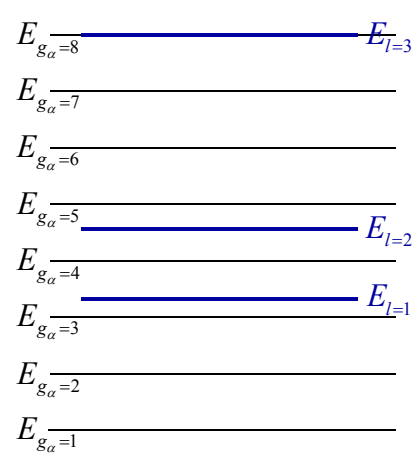

Figure 1. Three α energy emission energies overlaid on an evenly-spaced α energy grid. $E_{g_\alpha=8} = E_{l=3}$.

Equation (20) becomes

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial \sigma_{j,g_\alpha}} = \delta_{ij}\lambda_k \frac{N_k N_i}{N}\frac{1}{\varepsilon_{g_\alpha}}\left(\frac{E_{G_\alpha+1}-E_1}{G_\alpha}\right)$$
$$\times\left\{\sum_{\substack{l=1,\\ E_{g_\alpha,l}>E_{g_\alpha}}}^{L} f_{kl}^{\alpha} + \sum_{\substack{l=1,\\ E_{g_\alpha,l}=E_{g_\alpha}}}^{L} f_{kl}^{\alpha}\left(\frac{1}{2}+\frac{E_l-E_{g_\alpha,l}}{E_{g_\alpha+1,l}-E_{g_\alpha,l}}\left[1-\frac{1}{2}\right]\right) + \sum_{\substack{l=1,\\ E_{g_\alpha+1,l}=E_{g_\alpha}}}^{L} f_{kl}^{\alpha}\left(\frac{E_l-E_{g_\alpha,l}}{E_{g_\alpha+1,l}-E_{g_\alpha,l}}\left[\frac{1}{2}\right]\right)\right\}$$
$$= \delta_{ij}\lambda_k \frac{N_k N_i}{N}\frac{1}{\varepsilon_{g_\alpha}}\left(\frac{E_{G_\alpha+1}-E_1}{G_\alpha}\right)$$
$$\times\left\{\sum_{\substack{l=1,\\ E_{g_\alpha,l}>E_{g_\alpha}}}^{L} f_{kl}^{\alpha} + \sum_{\substack{l=1,\\ E_{g_\alpha,l}=E_{g_\alpha}}}^{L} f_{kl}^{\alpha}\frac{1}{2}\left(1+\frac{E_l-E_{g_\alpha,l}}{E_{g_\alpha+1,l}-E_{g_\alpha,l}}\right) + \sum_{\substack{l=1,\\ E_{g_\alpha+1,l}=E_{g_\alpha}}}^{L} f_{kl}^{\alpha}\frac{1}{2}\left(\frac{E_l-E_{g_\alpha,l}}{E_{g_\alpha+1,l}-E_{g_\alpha,l}}\right)\right\}. \tag{22}$$

The maximum energy $E_{G_\alpha+1}$ is the largest energy of the L α particles emitted from source isotope k. The stopping power ε_{g_α} at energy E_{g_α} and the energy group width do not depend on the index l.

The data file `tape3` contains, for each target isotope j, table values $(\hat{E}_{\hat{g}_\alpha}, \hat{\sigma}_{j,\hat{g}_\alpha})$. As an example, the data for O-17 are plotted in Figure 2. For each energy E_{g_α} on the α particle computational energy grid, the (α,n) cross section σ_{j,g_α} is interpolated linearly from the table values:

$$\sigma_{j,g_\alpha} = \frac{\hat{\sigma}_{j,\hat{g}_\alpha+1}-\hat{\sigma}_{j,\hat{g}_\alpha}}{\hat{E}_{\hat{g}_\alpha+1}-\hat{E}_{\hat{g}_\alpha}}E_{g_\alpha} + \frac{\hat{\sigma}_{j,\hat{g}_\alpha}\hat{E}_{\hat{g}_\alpha+1}-\hat{\sigma}_{j,\hat{g}_\alpha+1}\hat{E}_{\hat{g}_\alpha}}{\hat{E}_{\hat{g}_\alpha+1}-\hat{E}_{\hat{g}_\alpha}}, \quad \hat{E}_{\hat{g}_\alpha} \le E_{g_\alpha} \le \hat{E}_{\hat{g}_\alpha+1}. \tag{23}$$

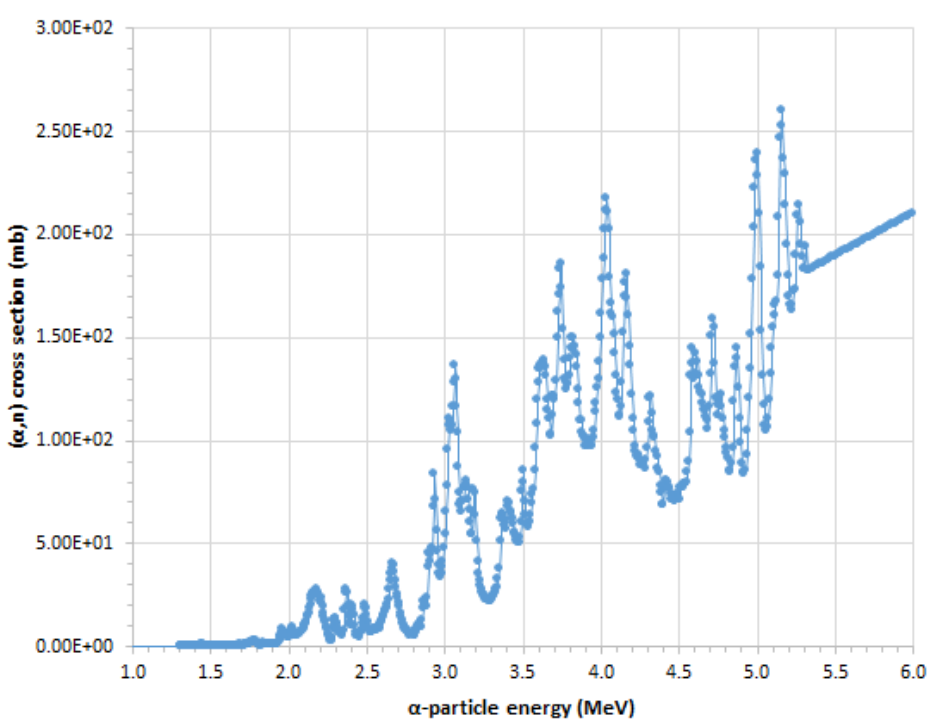

Figure 2. (α,n) neutron production cross section for O-17 as given in the SOURCES4C `tape3` data file.

If energy E_{g_α} on the computational energy grid is equal to an energy $\hat{E}_{\hat{g}_\alpha}$ on the table energy grid, Eq. (23) evaluates to

$$\sigma_{j,g_\alpha} = \hat{\sigma}_{j,\hat{g}_\alpha}. \tag{24}$$

The derivatives of σ_{j,g_α} with respect to the table values $\hat{\sigma}_{j,\hat{g}_\alpha+1}$ and $\hat{\sigma}_{j,\hat{g}_\alpha}$ are

$$\frac{\partial \sigma_{j,g_\alpha}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha+1}} = \frac{E_{g_\alpha} - \hat{E}_{\hat{g}_\alpha}}{\hat{E}_{\hat{g}_\alpha+1} - \hat{E}_{\hat{g}_\alpha}}, \hat{E}_{\hat{g}_\alpha} < E_{g_\alpha} < \hat{E}_{\hat{g}_\alpha+1}, \tag{25}$$

$$\frac{\partial \sigma_{j,g_\alpha}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha}} = \frac{\hat{E}_{\hat{g}_\alpha+1} - E_{g_\alpha}}{\hat{E}_{\hat{g}_\alpha+1} - \hat{E}_{\hat{g}_\alpha}}, \hat{E}_{\hat{g}_\alpha} < E_{g_\alpha} < \hat{E}_{\hat{g}_\alpha+1}, \tag{26}$$

and

$$\frac{\partial \sigma_{j,g_\alpha}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha}} = 1, \hat{E}_{\hat{g}_\alpha} = E_{g_\alpha}. \tag{27}$$

Finally, the derivatives of the source rate density with respect to the table values $\hat{\sigma}_{j,\hat{g}_\alpha+1}$ and $\hat{\sigma}_{j,\hat{g}_\alpha}$ are

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha+1}} = \frac{\partial Q_{(\alpha,n),k,i}}{\partial \sigma_{j,g_\alpha}} \frac{\partial \sigma_{j,g_\alpha}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha+1}} \tag{28a}$$

where the first factor on the right side is given by Eq. (22) and the second is given by Eq. (25), and

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha}} = \frac{\partial Q_{(\alpha,n),k,i}}{\partial \sigma_{j,g_\alpha}} \frac{\partial \sigma_{j,g_\alpha}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha}}, \tag{28b}$$

where the first factor on the right side is given by Eq. (22) and the second is given by Eq. (26) or (27). However, in general, a table value $\hat{\sigma}_{j,\hat{g}_\alpha}$ will affect at least the computational values σ_{j,g_α} to its left and right. Therefore, Eqs. (28a) and (28b) become the sum

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha}} = \sum_{g_\alpha \in \hat{g}_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \sigma_{j,g_\alpha}} \frac{\partial \sigma_{j,g_\alpha}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha}}, \tag{29}$$

where $g_\alpha \in \hat{g}_\alpha$ indicates all of the computational indices g_α affected by table index $\hat{g}_\alpha$. For $E_{g_\alpha} < \hat{E}_{\hat{g}_\alpha}$, Eq. (25) is used, but it is written

$$\frac{\partial \sigma_{j,g_\alpha}}{\partial \hat{\sigma}_{j,\hat{g}_\alpha}} = \frac{E_{g_\alpha} - \hat{E}_{\hat{g}_\alpha-1}}{\hat{E}_{\hat{g}_\alpha} - \hat{E}_{\hat{g}_\alpha-1}}, \hat{E}_{\hat{g}_\alpha-1} < E_{g_\alpha} < \hat{E}_{\hat{g}_\alpha}; \tag{30}$$

for $E_{g_\alpha} > \hat{E}_{\hat{g}_\alpha}$, Eq. (26) is used; for $E_{g_\alpha} = \hat{E}_{\hat{g}_\alpha}$, Eq. (27) is used.

IV. Derivative of the (α,n) Source Rate Density with Respect to the Stopping Power

In the SOURCES4C source code and manual, the stopping power is sometimes called the stopping cross section. Here we call it the stopping power. From Eq. (10), the derivative of $Q_{(\alpha,n),k,i}$ with respect to the stopping power ε_{j,g_α} for isotope *j* in α energy group g_α is

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} = \lambda_k N_k \sum_{l=1}^{L} f_{kl}^{\alpha} \frac{\partial P_i(E_l)}{\partial \varepsilon_{j,g_\alpha}}. \tag{31}$$

Accounting for the interpolation at α emission energies below $E_{G_\alpha+1}$, i.e. using Eq. (11), the derivative is

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} = \lambda_k N_k \sum_{l=1}^{L} f_{kl}^{\alpha} \left\{ \frac{\partial P_i(E_{g_\alpha,l})}{\partial \varepsilon_{j,g_\alpha}} + \frac{E_l - E_{g_\alpha,l}}{E_{g_\alpha+1,l} - E_{g_\alpha,l}} \left[\frac{\partial P_i(E_{g_\alpha+1,l})}{\partial \varepsilon_{j,g_\alpha}} - \frac{\partial P_i(E_{g_\alpha,l})}{\partial \varepsilon_{j,g_\alpha}} \right] \right\}. \tag{32}$$

The derivation of the derivative of $Q_{(\alpha,n),k,i}$ with respect to the stopping power follows exactly the derivation of Eq. (22) in Sec. III. The derivative of $1/\varepsilon_{g_\alpha}$ with respect to ε_{j,g_α} is needed; using Eq. (8), it is

$$\frac{\partial (1/\varepsilon_{g_\alpha})}{\partial \varepsilon_{j,g_\alpha}} = \frac{\partial}{\partial \varepsilon_{j,g_\alpha}} \left(\frac{N}{\sum_{j=1}^{J} N_j \varepsilon_{j,g_\alpha}} \right) = -\frac{N N_j}{\left(\sum_{j=1}^{J} N_j \varepsilon_{j,g_\alpha} \right)^2} = -\frac{N_j}{N \varepsilon_{g_\alpha}^2}. \tag{33}$$

The derivative of $Q_{(\alpha,n),k,i}$ with respect to the stopping power is

$$\begin{aligned} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} &= -\lambda_k \frac{N_k N_i N_j}{N^2} \frac{\sigma_{i,g_\alpha}}{\varepsilon_{g_\alpha}^2} \left(\frac{E_{G_\alpha+1} - E_1}{G_\alpha} \right) \\ &\times \left\{ \sum_{\substack{l=1,\\ E_{g_\alpha,l} > E_{g_\alpha}}}^{L} f_{kl}^{\alpha} + \sum_{\substack{l=1,\\ E_{g_\alpha,l} = E_{g_\alpha}}}^{L} f_{kl}^{\alpha} \frac{1}{2} \left(1 + \frac{E_l - E_{g_\alpha,l}}{E_{g_\alpha+1,l} - E_{g_\alpha,l}} \right) + \sum_{\substack{l=1,\\ E_{g_\alpha+1,l} = E_{g_\alpha}}}^{L} f_{kl}^{\alpha} \frac{1}{2} \left(\frac{E_l - E_{g_\alpha,l}}{E_{g_\alpha+1,l} - E_{g_\alpha,l}} \right) \right\}. \end{aligned} \tag{34}$$

The maximum energy $E_{G_\alpha+1}$ is the largest energy of the *L* α particles emitted from source isotope *k*. The stopping power ε_{g_α} and (α,n) cross section σ_{i,g_α} at energy E_{g_α} and the energy group width do not depend on the index *l*.

The stopping power for isotope *j* at α-particle energy E_{g_α} is the sum of a nuclear component and an electronic component:

$$\varepsilon_{j,g_\alpha} = \left[\varepsilon_{j,g_\alpha} \right]_{nuclear} + \left[\varepsilon_{j,g_\alpha} \right]_{electronic}. \tag{35}$$

The two components depend on the α-particle energy E_{g_α} but are otherwise independent. SOURCES4C computes the stopping power using data that is hard-coded in the source and data that is read from data file `tape2`.

The nuclear component uses the coefficient

$$W_{rep} \equiv \frac{b_1 A_j E_{g_\alpha}}{Z_\alpha Z_j \left(A_\alpha + A_j \right) \sqrt{Z_\alpha^{2/3} + Z_j^{2/3}}}, \tag{36}$$

where

Z_α, Z_j = nuclear charge of the α particle (2.0) and isotope *j*
A_α, A_j = atomic mass of the α particle (4.0) and isotope *j*
b_1 = a coefficient, coded in the source, given in Table I.

Table I. Coefficients for the Nuclear Component of the Stopping Power.[(a)]

Coefficient	Value[(b)]
b_1	32,530
b_2	1.593
b_3	1.7
b_4	6.8
b_5	3.4
b_6	0.47

(a) Not dependent on isotope. Hard-coded in the SOURCES4C source.
(b) Units are not yet known to the author.

The equation used for the nuclear component depends on the value of W_{rep} as follows:

$$\left[\varepsilon_{j,g_\alpha}\right]_{nuclear} = \begin{cases} b_2\sqrt{W_{rep}}, W_{rep} < 0.001 \\ \dfrac{b_3\sqrt{W_{rep}}\ln\left(W_{rep}+e\right)}{1+b_4W_{rep}+b_5W_{rep}^{3/2}}, 0.001 \le W_{rep} < 10 \\ \dfrac{\ln\left(b_6W_{rep}\right)}{2W_{rep}}, 10 \le W_{rep}, \end{cases} \tag{37}$$

where the coefficients b_2 through b_6 are the values given in Table I hard-coded in the source.

The derivative of W_{rep} with respect to b_1 is

$$\frac{\partial W_{rep}}{\partial b_1} = \frac{A_jE_{g_\alpha}}{Z_\alpha Z_j\left(A_\alpha + A_j\right)\sqrt{Z_\alpha^{2/3}+Z_j^{2/3}}} = \frac{W_{rep}}{b_1}. \tag{38}$$

The derivative of ε_{j,g_α} with respect to W_{rep} is

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial W_{rep}} = \frac{b_2}{2\sqrt{W_{rep}}}, W_{rep} < 0.001, \tag{39}$$

$$\begin{aligned} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial W_{rep}} &= \frac{\frac{1}{2}b_3(W_{rep})^{-1/2}\ln\left(W_{rep}+e\right)}{1+b_4W_{rep}+b_5W_{rep}^{3/2}} + \frac{b_3\sqrt{W_{rep}}}{(1+b_4W_{rep}+b_5W_{rep}^{3/2})}\frac{1}{(W_{rep}+e)} \\ &\quad - \frac{b_3\sqrt{W_{rep}}\ln\left(W_{rep}+e\right)}{(1+b_4W_{rep}+b_5W_{rep}^{3/2})^2}(b_4+\tfrac{3}{2}b_5W_{rep}^{1/2}), 0.001 \le W_{rep} < 10 \\ &= \frac{b_3\sqrt{W_{rep}}}{1+b_4W_{rep}+b_5W_{rep}^{3/2}}\left\{\frac{\ln\left(W_{rep}+e\right)}{2W_{rep}} + \frac{1}{W_{rep}+e}\right. \\ &\quad \left. - \frac{(b_4+\frac{3}{2}b_5\sqrt{W_{rep}})\ln\left(W_{rep}+e\right)}{(1+b_4W_{rep}+b_5W_{rep}^{3/2})}\right\}, 0.001 \le W_{rep} < 10, \end{aligned} \tag{40}$$

and

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial W_{rep}} = \frac{1}{2W_{rep}^2} - \frac{\ln\left(b_6 W_{rep}\right)}{2W_{rep}^2} = \frac{1}{2W_{rep}^2}\left[1 - \ln\left(b_6 W_{rep}\right)\right], 10 \le W_{rep}. \tag{41}$$

The derivative of ε_{j,g_α} with respect to b_1 is

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_1} = \frac{\partial \varepsilon_{j,g_\alpha}}{\partial W_{rep}}\frac{\partial W_{rep}}{\partial b_1} = \frac{b_2}{2\sqrt{W_{rep}}}\frac{W_{rep}}{b_1} = \frac{b_2}{2b_1}\sqrt{W_{rep}}, W_{rep} < 0.001, \tag{42}$$

$$\begin{aligned}\frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_1} = \frac{\partial \varepsilon_{j,g_\alpha}}{\partial W_{rep}}\frac{\partial W_{rep}}{\partial b_1} &= \frac{b_3\sqrt{W_{rep}}}{1 + b_4 W_{rep} + b_5 W_{rep}^{3/2}}\left\{\frac{\ln\left(W_{rep} + e\right)}{2W_{rep}} + \frac{1}{W_{rep} + e}\right. \\ &\left. - \frac{(b_4 + \frac{3}{2}b_5\sqrt{W_{rep}})\ln\left(W_{rep} + e\right)}{(1 + b_4 W_{rep} + b_5 W_{rep}^{3/2})}\right\}\frac{W_{rep}}{b_1}, 0.001 \le W_{rep} < 10 \\ &= \frac{b_3 W_{rep}^{3/2}}{b_1(1 + b_4 W_{rep} + b_5 W_{rep}^{3/2})}\left\{\frac{\ln\left(W_{rep} + e\right)}{2W_{rep}} + \frac{1}{W_{rep} + e}\right. \\ &\left. - \frac{(b_4 + \frac{3}{2}b_5\sqrt{W_{rep}})\ln\left(W_{rep} + e\right)}{(1 + b_4 W_{rep} + b_5 W_{rep}^{3/2})}\right\}, 0.001 \le W_{rep} < 10,\end{aligned} \tag{43}$$

and

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_1} = \frac{\partial \varepsilon_{j,g_\alpha}}{\partial W_{rep}}\frac{\partial W_{rep}}{\partial b_1} = \frac{1}{2W_{rep}^2}\left[1 - \ln\left(b_6 W_{rep}\right)\right]\frac{W_{rep}}{b_1} = \frac{1}{2b_1 W_{rep}}\left[1 - \ln\left(b_6 W_{rep}\right)\right], 10 \le W_{rep}. \tag{44}$$

The derivatives of ε_{j,g_α} with respect to b_2 through b_6 are

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_2} = \sqrt{W_{rep}}, W_{rep} < 0.001, \tag{45}$$

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_3} = \frac{\sqrt{W_{rep}}\ln\left(W_{rep} + e\right)}{1 + b_4 W_{rep} + b_5 W_{rep}^{3/2}}, 0.001 \le W_{rep} < 10, \tag{46}$$

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_4} = -\frac{b_3 W_{rep}^{3/2}\ln\left(W_{rep} + e\right)}{(1 + b_4 W_{rep} + b_5 W_{rep}^{3/2})^2}, 0.001 \le W_{rep} < 10, \tag{47}$$

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_5} = -\frac{b_3 W_{rep}^{2}\ln\left(W_{rep} + e\right)}{(1 + b_4 W_{rep} + b_5 W_{rep}^{3/2})^2}, 0.001 \le W_{rep} < 10, \tag{48}$$

and

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_6} = \frac{1}{2W_{rep} b_6}, 10 \le W_{rep}. \tag{49}$$

We assume that the *e*, 1, and 2 on the right sides of Eq. (37) are known constants.

The provenance and meaning of the coefficients in Table I are not yet known to this author. It is possible that b_4 and b_5 are identically $4b_3$ and $2b_3$, respectively, in which case Eq. (46) becomes

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_3} = \frac{\sqrt{W_{rep}}\ln\left(W_{rep}+e\right)}{1+4b_3W_{rep}+2b_3W_{rep}^{3/2}} - \frac{b_3\sqrt{W_{rep}}\ln\left(W_{rep}+e\right)}{(1+4b_3W_{rep}+2b_3W_{rep}^{3/2})^2}(4W_{rep}+2W_{rep}^{3/2}),\ 0.001 \le W_{rep} < 10, \tag{50}$$

and Eqs. (47) and (48) are not needed.

The equation for the electronic component of the stopping power depends on the α particle energy E_{g_α}. For $E_{g_\alpha} \le 30$ MeV,

$$\left[\varepsilon_{j,g_\alpha}\right]_{electronic} = \frac{s_{low}s_{high}}{s_{low}+s_{high}}, \tag{51}$$

where

$$s_{low} = c_{j,1}\left(1000E_{g_\alpha}\right)^{c_{j,2}} \tag{52}$$

and

$$s_{high} = \frac{c_{j,3}}{E_{g_\alpha}}\ln\left(1+\frac{c_{j,4}}{E_{g_\alpha}}+c_{j,5}E_{g_\alpha}\right). \tag{53}$$

The factor of 1000 in Eq. (52) is almost certainly a known constant to convert energy units. We assume the 1 in Eq. (53) is also a known constant. For $E_{g_\alpha} > 30$ MeV,

$$\left[\varepsilon_{j,g_\alpha}\right]_{electronic} = \exp\left(c_{j,6}+c_{j,7}E_x+c_{j,8}E_x^2+c_{j,9}E_x^3\right), \tag{54}$$

where

$$E_x = \ln\left(1/E_{g_\alpha}\right). \tag{55}$$

The coefficients $c_{j,1}$ through $c_{j,9}$ are given in the data file `tape2`.

The derivatives of ε_{j,g_α} with respect to s_{low} and s_{high} are

$$\begin{aligned}\frac{\partial \varepsilon_{j,g_\alpha}}{\partial s_{low}} &= \frac{s_{high}}{s_{low}+s_{high}} - \frac{s_{low}s_{high}}{(s_{low}+s_{high})^2} \\ &= \frac{s_{high}(s_{low}+s_{high})}{(s_{low}+s_{high})^2} - \frac{s_{low}s_{high}}{(s_{low}+s_{high})^2} \\ &= \frac{s_{high}^2}{(s_{low}+s_{high})^2}\end{aligned} \tag{56}$$

and likewise

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial s_{high}} = \frac{s_{low}^2}{(s_{low}+s_{high})^2}. \tag{57}$$

The derivatives of s_{low} with respect to $c_{j,1}$ and $c_{j,2}$ are

$$\frac{\partial s_{low}}{\partial c_{j,1}} = \left(1000E_{g_\alpha}\right)^{c_{j,2}} = \frac{s_{low}}{c_{j,1}} \tag{58}$$

and

$$\frac{\partial s_{low}}{\partial c_{j,2}} = c_{j,1}\left(1000E_{g_\alpha}\right)^{c_{j,2}} \ln(1000E_{g_\alpha}) = s_{low}\ln(1000E_{g_\alpha}). \tag{59}$$

The derivatives of s_{high} with respect to $c_{j,3}$, $c_{j,4}$, and $c_{j,5}$ are

$$\frac{\partial s_{high}}{\partial c_{j,3}} = \frac{1}{E_{g_\alpha}}\ln\left(1+\frac{c_{j,4}}{E_{g_\alpha}}+c_{j,5}E_{g_\alpha}\right) = \frac{s_{high}}{c_{j,3}}, \tag{60}$$

$$\frac{\partial s_{high}}{\partial c_{j,4}} = \frac{c_{j,3}}{E_{g_\alpha}^2}\frac{1}{1+\frac{c_{j,4}}{E_{g_\alpha}}+c_{j,5}E_{g_\alpha}}, \tag{61}$$

and

$$\frac{\partial s_{high}}{\partial c_{j,5}} = \frac{c_{j,3}}{E_{g_\alpha}}\frac{E_{g_\alpha}}{1+\frac{c_{j,4}}{E_{g_\alpha}}+c_{j,5}E_{g_\alpha}} = \frac{c_{j,3}}{1+\frac{c_{j,4}}{E_{g_\alpha}}+c_{j,5}E_{g_\alpha}}. \tag{62}$$

The derivatives of ε_{j,g_α} with respect to $c_{j,1}$, $c_{j,2}$, $c_{j,3}$, $c_{j,4}$, and $c_{j,5}$ are

$$\begin{aligned}\frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,1}} &= \frac{\partial \varepsilon_{j,g_\alpha}}{\partial s_{low}}\frac{\partial s_{low}}{\partial c_{j,1}} = \frac{s_{high}^2}{(s_{low}+s_{high})^2}\frac{s_{low}}{c_{j,1}} \\ &= \frac{\left[\varepsilon_{j,g_\alpha}\right]_{electronic}^2}{s_{low}c_{j,1}},\ E_{g_\alpha} \le 30,\end{aligned} \tag{63}$$

$$\begin{aligned}\frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,2}} &= \frac{\partial \varepsilon_{j,g_\alpha}}{\partial s_{low}}\frac{\partial s_{low}}{\partial c_{j,2}} = \frac{s_{high}^2}{(s_{low}+s_{high})^2}s_{low}\ln(1000E_{g_\alpha}) \\ &= \frac{\left[\varepsilon_{j,g_\alpha}\right]_{electronic}^2}{s_{low}}\ln(1000E_{g_\alpha}),\ E_{g_\alpha} \le 30,\end{aligned} \tag{64}$$

$$\begin{aligned}\frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,3}} &= \frac{\partial \varepsilon_{j,g_\alpha}}{\partial s_{high}}\frac{\partial s_{high}}{\partial c_{j,3}} = \frac{s_{low}^2}{(s_{low}+s_{high})^2}\frac{s_{high}}{c_{j,3}} \\ &= \frac{\left[\varepsilon_{j,g_\alpha}\right]_{electronic}^2}{s_{high}c_{j,3}},\ E_{g_\alpha} \le 30,\end{aligned} \tag{65}$$

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,4}} = \frac{\partial \varepsilon_{j,g_\alpha}}{\partial s_{high}} \frac{\partial s_{high}}{\partial c_{j,4}} = \frac{s_{low}^2}{(s_{low}+s_{high})^2} \frac{c_{j,3}}{E_{g_\alpha}^2} \frac{1}{1+\frac{c_{j,4}}{E_{g_\alpha}}+c_{j,5}E_{g_\alpha}}$$

$$= \frac{\left[\varepsilon_{j,g_\alpha}\right]_{electronic}^2}{s_{high}^2} \frac{c_{j,3}}{E_{g_\alpha}^2} \frac{1}{1+\frac{c_{j,4}}{E_{g_\alpha}}+c_{j,5}E_{g_\alpha}}, \; E_{g_\alpha} \le 30, \tag{66}$$

and

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,5}} = \frac{\partial \varepsilon_{j,g_\alpha}}{\partial s_{high}} \frac{\partial s_{high}}{\partial c_{j,5}} = \frac{s_{low}^2}{(s_{low}+s_{high})^2} \frac{c_{j,3}}{1+\frac{c_{j,4}}{E_{g_\alpha}}+c_{j,5}E_{g_\alpha}}$$

$$= \frac{\left[\varepsilon_{j,g_\alpha}\right]_{electronic}^2}{s_{high}^2} \frac{c_{j,3}}{1+\frac{c_{j,4}}{E_{g_\alpha}}+c_{j,5}E_{g_\alpha}}, \; E_{g_\alpha} \le 30. \tag{67}$$

where $\left[\varepsilon_{j,g_\alpha}\right]_{electronic}$, s_{low}, and s_{high} are given by Eqs. (51), (52), and (53).

The derivatives of ε_{j,g_α} with respect to $c_{j,6}$, $c_{j,7}$, $c_{j,8}$, and $c_{j,9}$ are

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,6}} = \exp\left(c_{j,6}+c_{j,7}E_x+c_{j,8}E_x^2+c_{j,9}E_x^3\right) = \left[\varepsilon_{j,g_\alpha}\right]_{electronic}, \; 30 < E_{g_\alpha}, \tag{68}$$

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,7}} = E_x \exp\left(c_{j,6}+c_{j,7}E_x+c_{j,8}E_x^2+c_{j,9}E_x^3\right) = E_x\left[\varepsilon_{j,g_\alpha}\right]_{electronic}, \; 30 < E_{g_\alpha}, \tag{69}$$

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,8}} = E_x^2 \exp\left(c_{j,6}+c_{j,7}E_x+c_{j,8}E_x^2+c_{j,9}E_x^3\right) = E_x^2\left[\varepsilon_{j,g_\alpha}\right]_{electronic}, \; 30 < E_{g_\alpha}, \tag{70}$$

and

$$\frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,9}} = E_x^3 \exp\left(c_{j,6}+c_{j,7}E_x+c_{j,8}E_x^2+c_{j,9}E_x^3\right) = E_x^3\left[\varepsilon_{j,g_\alpha}\right]_{electronic}, \; 30 < E_{g_\alpha}, \tag{71}$$

where $\left[\varepsilon_{j,g_\alpha}\right]_{electronic}$ and E_x are given by Eqs. (54) and (55).

Finally, the derivatives of the source rate density with respect to b_1 through b_6 are

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial b_1} = \sum_{j=1}^{J}\sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_1}, \tag{72}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (42), (43), or (44),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial b_2} = \sum_{j=1}^{J}\sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_2}, \tag{73}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (45),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial b_3} = \sum_{j=1}^{J} \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_3}, \tag{74}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (46),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial b_4} = \sum_{j=1}^{J} \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_4}, \tag{75}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (47),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial b_5} = \sum_{j=1}^{J} \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_5}, \tag{76}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (48), and

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial b_6} = \sum_{j=1}^{J} \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial b_6}, \tag{77}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (49), and the derivatives of the source rate density with respect to $c_{j,1}$ through $c_{j,9}$ are

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial c_{j,1}} = \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,1}}, \tag{78}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (63),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial c_{j,2}} = \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,2}}, \tag{79}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (64),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial c_{j,3}} = \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,3}}, \tag{80}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (65),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial c_{j,4}} = \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,4}}, \tag{81}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (66),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial c_{j,5}} = \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,5}}, \tag{82}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (67),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial c_{j,6}} = \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,6}}, \tag{83}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (68),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial c_{j,7}} = \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,7}}, \tag{84}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (69),

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial c_{j,8}} = \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,8}}, \tag{85}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (70), and

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial c_{j,9}} = \sum_{g_\alpha=1}^{G_\alpha} \frac{\partial Q_{(\alpha,n),k,i}}{\partial \varepsilon_{j,g_\alpha}} \frac{\partial \varepsilon_{j,g_\alpha}}{\partial c_{j,9}}, \tag{86}$$

where the first factor on the right side is given by Eq. (34) and the second by Eq. (71). In Eqs. (72) through (86), J is the number of elements in the material (because all elements contribute to the stopping power).

V. Modification of SOURCES4C

The term in curly braces in Eqs. (22) and (34) is the same. It is computed once and stored in a new variable, `dqdd`.

A new output file called `sdata` is written. The derivatives $\partial Q_{(\alpha,n),k,i} / \partial \sigma_{j,g_\alpha}$, $g_\alpha = 1,\ldots,G_\alpha+1$, are written under the heading `dqdsig`. The values in the energy grid, $(E_{g_\alpha}, \sigma_{j,g_\alpha})$, are also written. The derivatives $\partial Q_{(\alpha,n),k,i} / \partial \hat{\sigma}_{j,\hat{g}_\alpha}$, $\hat{g}_\alpha = 1,\ldots,\hat{G}_\alpha$ (where $\hat{G}_\alpha$ is the number of entries in the data table), are written under the heading `dqdx`. $\hat{G}_\alpha$ is written with the label that is the variable in the code, `jps`. The table values $(\hat{E}_{\hat{g}_\alpha}, \hat{\sigma}_{j,\hat{g}_\alpha})$ are also written.

The derivatives $\partial Q_{(\alpha,n),k,i} / \partial \varepsilon_{j,g_\alpha}$, $g_\alpha = 1,\ldots,G_\alpha+1$, are written under the heading `dqde`. The values in the energy grid, $(E_{g_\alpha}, \varepsilon_{j,g_\alpha})$, are also written. The derivatives $\partial Q_{(\alpha,n),k,i} / \partial b_n$, $n = 1,\ldots,6$, are written under the heading `dqdb`. The derivatives $\partial Q_{(\alpha,n),k,i} / \partial c_{j,n}$, $n = 1,\ldots,9$, are written under the heading `dqdc`.

These modifications are applied only to the calculation of the (α,n) neutron source from a homogeneous material.

VI. Test Problem

The test material was PuO_2 with the composition given in Table II. Its mass density was 10 g/cm^3. One hundred α energy groups were used (G_α = input variable `nag` = 100), meaning there were 101 energy bin boundaries. The full SOURCES4C input file is listed in the appendix.

Both plutonium isotopes in Table II are α emitters but only O-17 is an (α,n) target. All four isotopes contribute to the material's stopping power. The (α,n) neutron source rate density due to each combination of source and target is given in Table III. Pu-239 emits α particles at three energies and Pu-240 emits α particles at seven energies.

Table II. PuO_2 Material Composition.

Isotope	Atom Density (atoms/cm^3)	Weight Fraction
Pu-239	2.1215058E+22	8.42143E-01
Pu-240	9.9966255E+20	3.98484E-02
O-16	4.4411615E+22	1.17958E-01
O-17	1.7816217E+19	5.02911E-05

Table III. (α,n) Neutron Source Rate Density.

Source/Target	$Q_{(\alpha,n),k,i}$ (neutrons/cm^3/s)
Pu-239/O-17	2.7534206E+01
Pu-240/O-17	4.7938064E+00

VI.A.1. Derivative of the (α,n) Source Rate Density with Respect to the (α,n) Cross Section

There are currently 1076 values in the $(\hat{E}_{\hat{g}_\alpha}, \hat{\sigma}_{j,\hat{g}_\alpha})$ table for O-17. They are plotted (up to 6 MeV; the maximum value is 10.524 MeV) in Figure 2. (The (α,n) threshold for O-17 is 1.31 MeV, and lower α energies are not used in this particular problem.)

Derivatives of the (α,n) neutron source rate with respect to the table values of $\hat{\sigma}_{j,\hat{g}_\alpha}$ for O-17 are compared with central differences in Table IV for the source/target combination Pu-239/O-17 and in Table V for the source/target combination Pu-240/O-17. Because there are only 101 energies in the problem energy grid, many of the 1076 table values have no effect on the interpolated problem values. The derivatives of these table values are zero. They are not shown in Tables IV and V; these only show the 201 non-zero derivatives. The central differences were obtained by perturbing the table values by ±10 mb (not a relative amount).

The relative differences between the derivatives of this report and the central differences are generally well within 0.01%. Occasional large differences occur when the derivative is very small (e.g., a difference of 0.177% for $\hat{g}_\alpha$ = 302 on Table IV).

Table IV. Derivatives with Respect to O-17 $\hat{\sigma}_{j,\hat{g}_\alpha}$, Pu-239/O-17.[(a)]

$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]	$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]
2	1.2266E-03	1.2266E-03	–0.002%	446	4.0759E-04	4.0760E-04	0.003%
21	8.9290E-04	8.9290E-04	0.000%	447	3.3854E-03	3.3855E-03	0.001%
22	1.5837E-03	1.5837E-03	0.000%	453	2.6080E-03	2.6080E-03	0.000%
31	9.4127E-04	9.4125E-04	–0.002%	454	1.2089E-03	1.2089E-03	–0.002%
32	1.5594E-03	1.5594E-03	0.001%	459	1.0428E-03	1.0428E-03	0.000%
41	1.4259E-03	1.4259E-03	–0.001%	460	2.7977E-03	2.7978E-03	0.001%
42	1.0995E-03	1.0995E-03	–0.001%	466	3.5550E-03	3.5550E-03	0.000%
51	2.0510E-03	2.0510E-03	–0.001%	467	3.0913E-04	3.0915E-04	0.007%
52	4.9966E-04	4.9965E-04	–0.002%	472	2.2114E-03	2.2115E-03	0.001%
60	3.7655E-04	3.7655E-04	0.001%	473	1.6761E-03	1.6761E-03	0.000%
61	2.1998E-03	2.1998E-03	–0.001%	478	1.0749E-03	1.0749E-03	0.000%
70	1.5516E-03	1.5516E-03	0.000%	479	2.8360E-03	2.8360E-03	0.000%
71	1.0509E-03	1.0509E-03	–0.002%	484	2.3729E-05	2.3750E-05	0.088%
79	6.0147E-04	6.0145E-04	–0.003%	485	3.9103E-03	3.9103E-03	–0.001%
80	2.0275E-03	2.0276E-03	0.000%	491	3.0956E-03	3.0957E-03	0.000%
89	2.6377E-03	2.6377E-03	0.001%	492	8.6149E-04	8.6150E-04	0.002%
90	1.8137E-05	1.8150E-05	0.070%	497	2.3047E-03	2.3047E-03	–0.001%
107	2.3720E-03	2.3720E-03	0.001%	498	1.6754E-03	1.6754E-03	–0.001%
108	3.1090E-04	3.1090E-04	0.000%	503	1.6668E-03	1.6668E-03	0.000%
125	2.4753E-03	2.4753E-03	0.001%	504	2.3361E-03	2.3362E-03	0.000%
126	2.3488E-04	2.3490E-04	0.008%	509	1.0697E-03	1.0697E-03	0.002%
138	2.9492E-04	2.9490E-04	–0.006%	510	2.9560E-03	2.9560E-03	0.000%
139	2.4427E-03	2.4427E-03	0.000%	516	1.0431E-03	1.0432E-03	0.001%
147	1.0106E-03	1.0106E-03	–0.001%	517	3.0052E-03	3.0052E-03	0.000%
148	1.7547E-03	1.7547E-03	0.000%	522	4.7196E-04	4.7195E-04	–0.002%
156	1.9309E-03	1.9310E-03	0.001%	523	3.5988E-03	3.5989E-03	0.000%

Table IV (cont.) Derivatives with Respect to O-17 $\hat{\sigma}_{j,\hat{g}_\alpha}$, Pu-239/O-17.[a]

$\hat{g}_\alpha$	This Report	Central Diff.	Difference[b]	$\hat{g}_\alpha$	This Report	Central Diff.	Difference[b]
157	8.6200E-04	8.6200E-04	0.000%	528	1.8520E-04	1.8520E-04	–0.001%
164	3.1225E-04	3.1225E-04	0.001%	529	3.9080E-03	3.9080E-03	0.000%
165	2.5085E-03	2.5085E-03	–0.001%	534	1.3504E-04	1.3505E-04	0.007%
173	1.7637E-03	1.7637E-03	–0.002%	535	3.9805E-03	3.9805E-03	0.000%
174	1.0849E-03	1.0849E-03	–0.002%	540	2.2240E-04	2.2240E-04	–0.001%
181	6.2562E-04	6.2560E-04	–0.004%	541	3.9153E-03	3.9153E-03	0.000%
182	2.2508E-03	2.2508E-03	0.000%	546	4.2732E-04	4.2735E-04	0.006%
190	2.5598E-03	2.5598E-03	0.000%	547	3.7325E-03	3.7325E-03	0.000%
191	3.4456E-04	3.4455E-04	–0.002%	552	6.4121E-04	6.4120E-04	–0.001%
198	1.8167E-03	1.8167E-03	0.000%	553	3.5406E-03	3.5406E-03	–0.001%
199	1.1155E-03	1.1155E-03	–0.002%	558	1.1758E-03	1.1758E-03	0.000%
206	1.2522E-03	1.2522E-03	–0.002%	559	3.0279E-03	3.0279E-03	–0.001%
207	1.7078E-03	1.7078E-03	–0.001%	564	1.7158E-03	1.7158E-03	0.000%
215	1.0263E-03	1.0263E-03	–0.001%	565	2.5097E-03	2.5097E-03	–0.001%
216	1.9616E-03	1.9616E-03	0.001%	570	2.5695E-03	2.5696E-03	0.001%
223	9.5117E-04	9.5115E-04	–0.002%	571	1.6776E-03	1.6777E-03	0.001%
224	2.0644E-03	2.0645E-03	0.001%	576	3.3809E-03	3.3809E-03	0.000%
231	1.0449E-03	1.0449E-03	–0.001%	577	8.8790E-04	8.8790E-04	0.000%
232	1.9984E-03	1.9984E-03	–0.001%	582	4.2789E-03	4.2789E-03	0.000%
239	1.4302E-03	1.4302E-03	0.000%	583	1.1357E-05	1.1350E-05	–0.058%
240	1.6407E-03	1.6408E-03	0.001%	587	1.0213E-03	1.0214E-03	0.002%
247	1.9703E-03	1.9704E-03	0.001%	588	3.2904E-03	3.2904E-03	0.000%
248	1.1281E-03	1.1281E-03	–0.002%	593	2.3258E-03	2.3258E-03	–0.001%
256	2.8979E-03	2.8979E-03	0.000%	594	2.0072E-03	2.0072E-03	0.000%
257	2.2792E-04	2.2795E-04	0.011%	599	3.6180E-03	3.6180E-03	0.000%
269	2.3232E-03	2.3232E-03	0.000%	600	7.3627E-04	7.3625E-04	–0.002%
270	8.2999E-04	8.3000E-04	0.001%	604	5.9068E-04	5.9070E-04	0.003%
280	1.5694E-03	1.5694E-03	0.000%	605	3.7847E-03	3.7848E-03	0.000%
281	1.6109E-03	1.6110E-03	0.000%	610	2.2632E-03	2.2633E-03	0.001%
288	2.8819E-03	2.8820E-03	0.000%	611	2.1333E-03	2.1333E-03	0.000%
289	3.2550E-04	3.2550E-04	0.001%	616	3.9604E-03	3.9604E-03	0.000%
295	1.4219E-03	1.4219E-03	0.000%	617	4.5711E-04	4.5710E-04	–0.003%
296	1.8125E-03	1.8125E-03	–0.001%	621	1.1879E-03	1.1879E-03	–0.002%
302	1.2079E-05	1.2100E-05	0.177%	622	3.2505E-03	3.2505E-03	0.000%
303	3.2492E-03	3.2492E-03	0.000%	627	2.9067E-03	2.9067E-03	0.000%
310	2.0334E-03	2.0334E-03	–0.001%	628	1.5525E-03	1.5525E-03	0.000%
311	1.2546E-03	1.2546E-03	0.002%	632	7.1679E-04	7.1680E-04	0.001%
317	8.3708E-04	8.3710E-04	0.002%	633	3.7632E-03	3.7632E-03	0.000%
318	2.4775E-03	2.4775E-03	0.000%	638	2.8790E-03	2.8791E-03	0.001%
325	3.2308E-03	3.2309E-03	0.000%	639	1.6216E-03	1.6216E-03	0.001%
326	1.1013E-04	1.1015E-04	0.020%	643	5.9209E-04	5.9210E-04	0.001%
332	2.6120E-03	2.6120E-03	0.000%	644	3.9291E-03	3.9291E-03	0.000%
333	7.5533E-04	7.5535E-04	0.003%	649	2.7557E-03	2.7557E-03	–0.001%
339	1.9418E-03	1.9418E-03	0.000%	650	1.7860E-03	1.7860E-03	0.000%
340	1.4516E-03	1.4517E-03	0.001%	654	7.5461E-04	7.5460E-04	–0.001%
346	1.4716E-03	1.4717E-03	0.001%	655	3.8076E-03	3.8076E-03	0.000%
347	1.9478E-03	1.9479E-03	0.001%	660	3.3007E-03	3.3007E-03	0.001%

Table IV (cont.) Derivatives with Respect to O-17 $\hat{\sigma}_{j,\hat{g}_\alpha}$, Pu-239/O-17.[(a)]

$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]	$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]
353	1.2493E-03	1.2493E-03	–0.001%	661	1.2819E-03	1.2819E-03	0.000%
354	2.1961E-03	2.1961E-03	0.000%	665	1.4210E-03	1.4211E-03	0.000%
360	1.1727E-03	1.1728E-03	0.001%	666	3.1818E-03	3.1818E-03	0.000%
361	2.2984E-03	2.2984E-03	–0.001%	671	4.3688E-03	4.3688E-03	0.000%
367	1.3275E-03	1.3275E-03	0.000%	672	2.5427E-04	2.5425E-04	–0.007%
368	2.1692E-03	2.1692E-03	0.000%	676	2.4589E-03	2.4590E-03	0.000%
374	1.6101E-03	1.6102E-03	0.001%	677	2.1843E-03	2.1843E-03	–0.001%
375	1.9120E-03	1.9121E-03	0.001%	681	6.1309E-04	6.1310E-04	0.002%
381	1.9669E-03	1.9669E-03	0.001%	682	4.0502E-03	4.0503E-03	0.001%
382	1.5806E-03	1.5806E-03	0.000%	687	3.7654E-03	3.7654E-03	0.000%
387	2.6500E-03	2.6501E-03	0.001%	688	9.1793E-04	9.1795E-04	0.002%
388	9.2262E-04	9.2260E-04	–0.002%	692	2.4201E-03	2.4201E-03	0.000%
393	3.4448E-03	3.4448E-03	0.000%	693	2.2832E-03	2.2833E-03	0.001%
394	1.5290E-04	1.5290E-04	–0.001%	697	1.1620E-03	1.1621E-03	0.001%
400	7.7368E-04	7.7370E-04	0.003%	698	3.5612E-03	3.5612E-03	0.000%
401	2.8489E-03	2.8489E-03	0.000%	703	4.4377E-03	4.4377E-03	0.000%
407	1.9027E-03	1.9027E-03	0.000%	704	3.0537E-04	3.0535E-04	–0.007%
408	1.7446E-03	1.7447E-03	0.000%	708	3.3364E-03	3.3364E-03	0.000%
414	3.0690E-03	3.0690E-03	0.001%	709	1.4264E-03	1.4264E-03	0.000%
415	6.0297E-04	6.0295E-04	–0.004%	713	2.2917E-03	2.2917E-03	–0.001%
420	7.9077E-04	7.9075E-04	–0.003%	714	2.4908E-03	2.4909E-03	0.001%
421	2.9057E-03	2.9057E-03	0.000%	718	1.0533E-03	1.0533E-03	0.002%
427	2.4583E-03	2.4583E-03	0.001%	719	3.6581E-03	3.6581E-03	0.000%
428	1.2625E-03	1.2625E-03	0.000%	723	1.5802E-04	1.5800E-04	–0.010%
433	4.2274E-04	4.2275E-04	0.002%	724	4.1785E-03	4.1785E-03	–0.001%
434	3.3223E-03	3.3223E-03	0.000%	729	1.7476E-03	1.7476E-03	0.000%
440	2.2095E-03	2.2095E-03	0.000%	730	2.7740E-04	2.7740E-04	0.002%
441	1.5596E-03	1.5596E-03	–0.001%				

(a) Only non-zero derivatives are presented.
(b) With respect to the central difference.

Table V. Derivatives with Respect to O-17 $\hat{\sigma}_{j,\hat{g}_\alpha}$, Pu-240/O-17.[(a)]

$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]	$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]
2	2.1357E-04	2.1357E-04	0.000%	447	8.8649E-05	8.8650E-05	0.001%
21	1.4196E-04	1.4196E-04	0.000%	448	5.7243E-04	5.7243E-04	0.000%
22	2.8927E-04	2.8927E-04	0.000%	454	4.5144E-04	4.5144E-04	0.000%
31	1.3800E-04	1.3800E-04	0.000%	455	2.1379E-04	2.1379E-04	–0.001%
32	2.9744E-04	2.9744E-04	0.000%	460	1.7052E-04	1.7053E-04	0.001%
41	2.0905E-04	2.0905E-04	–0.001%	461	4.9884E-04	4.9884E-04	0.000%
42	2.3070E-04	2.3070E-04	–0.001%	467	5.7102E-04	5.7102E-04	0.000%
51	3.0431E-04	3.0431E-04	0.000%	468	1.0246E-04	1.0246E-04	–0.002%
52	1.3986E-04	1.3986E-04	0.000%	473	3.5433E-04	3.5434E-04	0.000%
61	4.4754E-04	4.4754E-04	0.000%	474	3.2323E-04	3.2324E-04	0.001%
62	1.1217E-06	1.1200E-06	–0.147%	479	1.6316E-04	1.6316E-04	0.000%

Table V (cont.) Derivatives with Respect to O-17 $\hat{\sigma}_{j,\hat{g}_\alpha}$, Pu-240/O-17.[(a)]

$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]	$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]
70	1.9510E-04	1.9511E-04	0.000%	480	5.1848E-04	5.1848E-04	0.000%
71	2.5812E-04	2.5813E-04	0.000%	486	6.3240E-04	6.3241E-04	0.000%
79	1.4071E-05	1.4070E-05	–0.006%	487	5.3281E-05	5.3280E-05	–0.002%
80	4.4379E-04	4.4379E-04	–0.001%	492	4.6855E-04	4.6855E-04	0.000%
89	3.5469E-04	3.5469E-04	0.000%	493	2.2116E-04	2.2116E-04	0.000%
90	1.0785E-04	1.0785E-04	–0.001%	498	3.3685E-04	3.3685E-04	0.000%
107	2.6964E-04	2.6964E-04	–0.001%	499	3.5687E-04	3.5687E-04	0.000%
108	1.9763E-04	1.9763E-04	–0.001%	504	2.1585E-04	2.1586E-04	0.001%
125	2.4860E-04	2.4861E-04	0.000%	505	4.8185E-04	4.8185E-04	0.000%
126	2.2343E-04	2.2343E-04	0.000%	510	1.0942E-04	1.0942E-04	–0.002%
139	3.8992E-04	3.8992E-04	0.000%	511	5.9225E-04	5.9226E-04	0.000%
140	8.6913E-05	8.6915E-05	0.002%	517	2.4193E-05	2.4195E-05	0.010%
147	2.3645E-05	2.3645E-05	0.002%	518	6.8143E-04	6.8143E-04	0.000%
148	4.5801E-04	4.5801E-04	0.000%	524	6.8006E-04	6.8006E-04	0.000%
156	1.6961E-04	1.6961E-04	–0.002%	525	2.9491E-05	2.9490E-05	–0.002%
157	3.1688E-04	3.1688E-04	0.000%	530	6.5237E-04	6.5237E-04	0.000%
165	3.6017E-04	3.6017E-04	0.000%	531	6.1090E-05	6.1090E-05	0.001%
166	1.3118E-04	1.3118E-04	–0.002%	536	6.3422E-04	6.3423E-04	0.000%
173	1.2352E-04	1.2353E-04	0.001%	537	8.3121E-05	8.3120E-05	–0.001%
174	3.7268E-04	3.7268E-04	0.000%	542	6.1388E-04	6.1389E-04	0.000%
182	4.0860E-04	4.0861E-04	0.001%	543	1.0733E-04	1.0734E-04	0.001%
183	9.2471E-05	9.2470E-05	–0.001%	548	6.3784E-04	6.3785E-04	0.000%
190	2.1917E-04	2.1917E-04	0.000%	549	8.7228E-05	8.7230E-05	0.002%
191	2.8678E-04	2.8678E-04	–0.001%	554	7.2025E-04	7.2026E-04	0.000%
198	8.9555E-05	8.9555E-05	0.000%	555	8.6558E-06	8.6550E-06	–0.009%
199	4.2126E-04	4.2126E-04	0.000%	559	4.9071E-05	4.9070E-05	–0.001%
207	4.8852E-04	4.8853E-04	0.001%	560	6.8366E-04	6.8366E-04	0.000%
208	2.7152E-05	2.7150E-05	–0.007%	565	1.2945E-04	1.2945E-04	–0.001%
216	4.4192E-04	4.4192E-04	0.000%	566	6.0708E-04	6.0708E-04	0.000%
217	7.8611E-05	7.8610E-05	–0.001%	571	2.5594E-04	2.5594E-04	0.001%
224	4.2446E-04	4.2446E-04	0.000%	572	4.8438E-04	4.8438E-04	0.000%
225	1.0092E-04	1.0092E-04	–0.001%	577	3.8287E-04	3.8287E-04	0.000%
232	4.3239E-04	4.3239E-04	0.000%	578	3.6122E-04	3.6122E-04	0.000%
233	9.7818E-05	9.7820E-05	0.002%	583	5.5680E-04	5.5680E-04	0.000%
240	4.9288E-04	4.9289E-04	0.000%	584	1.9104E-04	1.9104E-04	0.001%
241	4.2147E-05	4.2145E-05	–0.005%	589	7.2106E-04	7.2106E-04	0.000%
247	3.6577E-05	3.6575E-05	–0.004%	590	3.0519E-05	3.0520E-05	0.005%
248	5.0326E-04	5.0326E-04	0.000%	594	2.0251E-04	2.0251E-04	–0.001%
256	1.7587E-04	1.7587E-04	–0.002%	595	5.5279E-04	5.5279E-04	0.000%
257	3.6876E-04	3.6876E-04	0.000%	600	3.8709E-04	3.8710E-04	0.001%
270	4.1967E-04	4.1967E-04	0.000%	601	3.7191E-04	3.7192E-04	0.001%
271	1.2973E-04	1.2973E-04	–0.002%	606	6.5707E-04	6.5708E-04	0.000%
281	4.8087E-04	4.8088E-04	0.001%	607	1.0562E-04	1.0562E-04	–0.002%
282	7.3270E-05	7.3270E-05	0.000%	611	1.4696E-04	1.4697E-04	0.001%
288	1.6601E-04	1.6601E-04	0.000%	612	6.1941E-04	6.1941E-04	0.000%
289	3.9287E-04	3.9287E-04	0.000%	617	4.3280E-04	4.3281E-04	0.000%
296	4.4675E-04	4.4675E-04	0.000%	618	3.3723E-04	3.3723E-04	0.000%

Table V (cont.) Derivatives with Respect to O-17 $\hat{\sigma}_{j,\hat{g}_\alpha}$, Pu-240/O-17.[(a)]

$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]	$\hat{g}_\alpha$	This Report	Central Diff.	Difference[(b)]
297	1.1683E-04	1.1684E-04	0.001%	623	7.3445E-04	7.3446E-04	0.000%
303	1.8274E-04	1.8274E-04	–0.001%	624	3.9229E-05	3.9230E-05	0.003%
304	3.8553E-04	3.8553E-04	0.000%	628	3.0432E-04	3.0433E-04	0.000%
311	5.2603E-04	5.2604E-04	0.000%	629	4.7299E-04	4.7299E-04	0.000%
312	4.6895E-05	4.6895E-05	0.000%	634	6.4037E-04	6.4037E-04	0.000%
318	3.0833E-04	3.0834E-04	0.001%	635	1.4057E-04	1.4057E-04	0.001%
319	2.6924E-04	2.6924E-04	0.000%	639	1.8718E-04	1.8719E-04	0.000%
325	1.5029E-04	1.5029E-04	0.000%	640	5.9736E-04	5.9736E-04	0.000%
326	4.3189E-04	4.3190E-04	0.000%	645	5.8656E-04	5.8656E-04	0.000%
332	1.3806E-06	1.3800E-06	–0.047%	646	2.0157E-04	2.0157E-04	0.000%
333	5.8539E-04	5.8540E-04	0.000%	650	1.4755E-04	1.4755E-04	–0.001%
340	4.8312E-04	4.8312E-04	0.000%	651	6.4417E-04	6.4417E-04	0.000%
341	1.0823E-04	1.0823E-04	–0.002%	656	5.8487E-04	5.8487E-04	0.000%
347	3.9882E-04	3.9882E-04	–0.001%	657	2.1041E-04	2.1041E-04	0.001%
348	1.9707E-04	1.9707E-04	–0.001%	661	2.3096E-04	2.3096E-04	–0.001%
354	3.5455E-04	3.5456E-04	0.000%	662	5.6788E-04	5.6788E-04	0.000%
355	2.4585E-04	2.4585E-04	0.000%	667	7.1911E-04	7.1912E-04	0.000%
361	3.3312E-04	3.3313E-04	0.000%	668	8.3261E-05	8.3260E-05	–0.001%
362	2.7177E-04	2.7177E-04	0.000%	672	3.6345E-04	3.6345E-04	0.000%
368	3.3366E-04	3.3366E-04	0.000%	673	4.4245E-04	4.4246E-04	0.001%
369	2.7571E-04	2.7571E-04	0.001%	677	4.7881E-05	4.7880E-05	–0.003%
375	3.8582E-04	3.8582E-04	0.000%	678	7.6154E-04	7.6154E-04	0.000%
376	2.2799E-04	2.2799E-04	0.000%	683	5.7683E-04	5.7684E-04	0.000%
382	4.3360E-04	4.3360E-04	0.000%	684	2.3609E-04	2.3610E-04	0.001%
383	1.8463E-04	1.8463E-04	0.000%	688	2.7457E-04	2.7458E-04	0.000%
388	5.5102E-04	5.5102E-04	0.000%	689	5.4184E-04	5.4185E-04	0.000%
389	7.1601E-05	7.1600E-05	–0.002%	694	8.1698E-04	8.1698E-04	0.000%
393	4.1874E-05	4.1875E-05	0.003%	695	2.9202E-06	2.9200E-06	–0.006%
394	5.8511E-04	5.8512E-04	0.000%	699	6.1656E-04	6.1656E-04	0.000%
401	1.9075E-04	1.9076E-04	0.001%	700	2.0681E-04	2.0681E-04	0.000%
402	4.4058E-04	4.4058E-04	0.000%	704	3.5225E-04	3.5225E-04	0.000%
408	3.8499E-04	3.8499E-04	0.000%	705	4.7458E-04	4.7458E-04	0.000%
409	2.5066E-04	2.5067E-04	0.001%	709	1.7614E-04	1.7615E-04	0.002%
415	5.7791E-04	5.7791E-04	0.000%	710	6.5385E-04	6.5385E-04	0.000%
416	6.2042E-05	6.2045E-05	0.004%	715	8.0327E-04	8.0327E-04	0.000%
421	1.8747E-04	1.8747E-04	–0.002%	716	2.9803E-05	2.9805E-05	0.007%
422	4.5675E-04	4.5676E-04	0.001%	720	5.5651E-04	5.5651E-04	0.000%
428	4.6690E-04	4.6690E-04	0.000%	721	2.6252E-04	2.6252E-04	0.000%
429	1.8157E-04	1.8157E-04	–0.001%	725	3.5710E-04	3.5710E-04	0.000%
434	8.8001E-05	8.8000E-05	–0.001%	726	3.5136E-04	3.5136E-04	0.000%
435	5.6469E-04	5.6470E-04	0.000%	730	8.7193E-05	8.7195E-05	0.003%
441	3.8968E-04	3.8969E-04	0.000%	731	2.2006E-04	2.2006E-04	–0.001%
442	2.6721E-04	2.6721E-04	–0.001%				

(a) Only non-zero derivatives are presented.
(b) With respect to the central difference.

VI.A.2. Derivative of the (α,n) Source Rate Density with Respect to the Stopping Power Data

The stopping powers for plutonium and oxygen are shown in Figure 3. (The (α,n) threshold for O-17 is 1.31 MeV, and lower α energies are not used in this particular problem.) Derivatives of the (α,n) neutron source rate with respect to b_1 and b_6 are compared with central differences in Table VI. The central differences were obtained by perturbing b_1 by ±2% and b_6 by ±5%. In this problem, derivatives with respect to b_2 through b_5 are all zero.

Table VI. Derivatives with Respect to b_n Parameters.

Parameter	Source/Target	This Report	Central Diff.	Difference[(a)]
b_1	Pu-239/O-17	7.995620E-08	7.992622E-08	–0.037%
	Pu-240/O-17	1.391777E-08	1.391024E-08	–0.054%
b_6	Pu-239/O-17	–1.579531E-03	–1.574468E-03	–0.321%
	Pu-240/O-17	–2.748554E-04	–2.744681E-04	–0.141%

(a) With respect to the central difference.

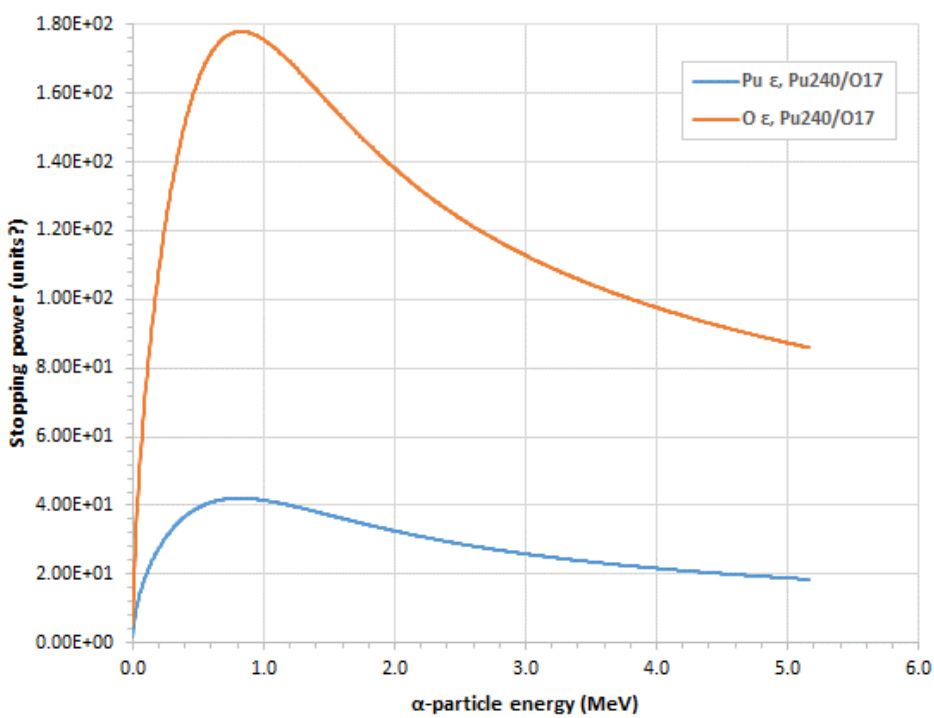

Figure 3. Stopping power for plutonium and oxygen in the test problem, computed on the Pu-240/O-17 energy grid (with a minimum energy of 0.001 MeV, not the energy used in SOURCES4C for this problem).

The comparison with the central difference for b_6 in Table VI is not completely satisfactory. The source rate density is plotted as a function of b_6 (for the Pu-239/O-17 source/target combination) in Figure 4. It is a (nearly perfect!) logarithmic function whose derivative at the unperturbed value of b_6 is –7.4234843E-04/0.47 = –1.579465E-03. The difference between the derivative of this report and the fit is 0.004%.

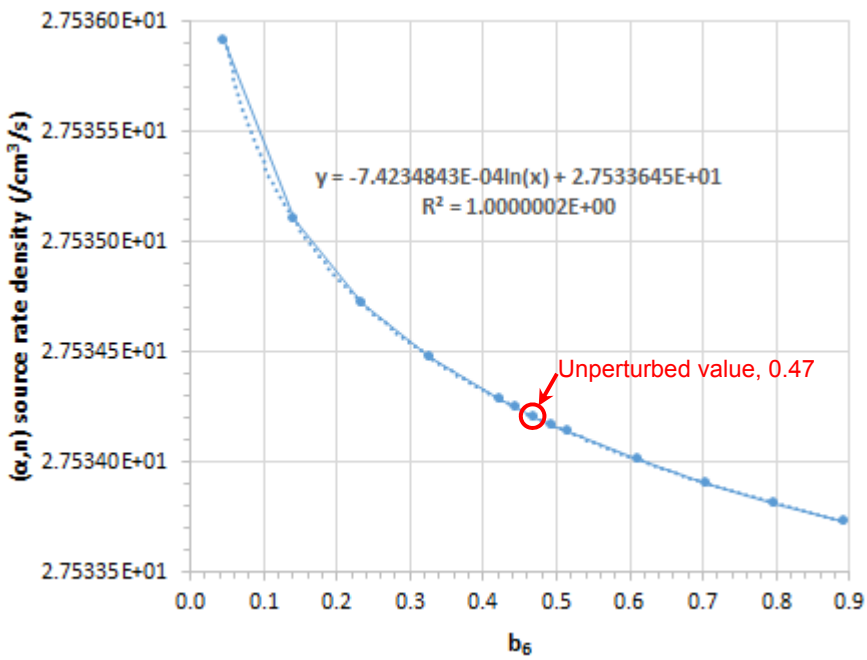

Figure 4. $Q_{(\alpha,n),k,i}$ as a function of b_6.

Derivatives of the (α,n) neutron source rate with respect to $c_{j,1}$ through $c_{j,5}$ are compared with central differences in Table VI. The central differences were all obtained by perturbing the $c_{j,n}$ parameters by ±1%. In this problem, derivatives with respect to $c_{j,6}$ through $c_{j,9}$ are all zero. The differences are all within 0.03%.

Table VII. Derivatives with Respect to $c_{j,n}$ Parameters.

Parameter	Element	Source/Target	This Report	Central Diff.	Difference[(a)]
$c_{j,1}$	Pu	Pu-239/O-17	–7.487849E-01	–7.488392E-01	0.007%
		Pu-240/O-17	–1.301851E-01	–1.301954E-01	0.008%
	O	Pu-239/O-17	–5.645723E-01	–5.646218E-01	0.009%
		Pu-240/O-17	–9.817674E-02	–9.818503E-02	0.008%
$c_{j,2}$	Pu	Pu-239/O-17	–1.093845E+01	–1.093984E+01	0.013%
		Pu-240/O-17	–1.902038E+00	–1.902281E+00	0.013%
	O	Pu-239/O-17	–2.405237E+01	–2.405912E+01	0.028%
		Pu-240/O-17	–4.183182E+00	–4.184356E+00	0.028%
$c_{j,3}$	Pu	Pu-239/O-17	–1.922038E-01	–1.922070E-01	0.002%
		Pu-240/O-17	–3.346817E-02	–3.346874E-02	0.002%
	O	Pu-239/O-17	–5.493044E-02	–5.493340E-02	0.005%
		Pu-240/O-17	–9.566128E-03	–9.566650E-03	0.005%
$c_{j,4}$	Pu	Pu-239/O-17	–3.927362E-02	–3.927493E-02	0.003%
		Pu-240/O-17	–6.826870E-03	–6.826772E-03	–0.001%
	O	Pu-239/O-17	–5.292367E-01	–5.292311E-01	–0.001%
		Pu-240/O-17	–9.198995E-02	–9.198907E-02	–0.001%
$c_{j,5}$	Pu	Pu-239/O-17	–6.404032E-01	–6.404244E-01	0.003%
		Pu-240/O-17	–1.115526E-01	–1.115567E-01	0.004%
	O	Pu-239/O-17	–8.585507E+00	–8.585890E+00	0.004%
		Pu-240/O-17	–1.495454E+00	–1.495520E+00	0.004%

(a) With respect to the central difference.

VII. Summary and Future Work

Derivatives of the (α,n) neutron source rate density with respect to the (α,n) cross section and stopping power data that SOURCES4C reads from the `tape2` and `tape3` files can now be output from a standard SOURCES4C calculation. These derivatives can be used to evaluate the effect of uncertainty in the nuclear data on the uncertainty in the (α,n) neutron source rate densities. The nuclear data for (α,n) reactions is still being evaluated and improved.[7] It is hoped that the new SOURCES4C capability will be useful in those efforts.

The next step that is needed for full utility of this capability is to determine the derivatives of the nuclear data passed to SOURCES4C in the `tape2` and `tape3` files with respect to all of the evaluated parameters used to compute them. In other words, we need $\partial\hat{\sigma}_{i,\hat{g}_\alpha}/\partial\beta_n$, $n = 1,\ldots,X$; $\partial b_m/\partial\beta_n$, $m = 1,\ldots,6$, $n = X+1,\ldots,X+Y$; and $\partial c_{j,m}/\partial\beta_n$, $m = 1,\ldots,9$, $n = X+Y+1,\ldots,X+Y+Z$. In this notation, β represents the parameters on which the nuclear data depend, and X, Y, and Z are the number of parameters on which $\hat{\sigma}_{i,\hat{g}_\alpha}$, b_m, and $c_{j,m}$ depend.

According to Ref. 3, the ORIGEN isotope production and depletion code[8] has implemented the methods of SOURCES4C. Therefore, the equations of this report, and perhaps even the code that was implemented in SOURCES4C for this work, can be applied to ORIGEN.

This work did not consider the derivative of the (α,n) neutron spectrum with respect to the nuclear data. If there is interest, that can be done. Until then, the insight gained in Ref. 1 can be used as an approximation. In Ref. 1, it was found that a good approximation for the derivative of the (α,n) neutron spectrum with respect to an isotope density (for a given source/target combination) is the derivative of the (α,n) neutron source rate density multiplied by the (α,n) neutron source spectrum (for the given source/target combination).

It should be noted that the derivatives with respect to some of the nuclear data were not tested in the problem presented here. Also, the quantities used in this report should all be given appropriate units—although it is interesting that such a level of detail is not needed to compute derivatives correctly!

Contact the author for access to the modified SOURCES4C source code.

Acknowledgments

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APPENDIX A
SOURCES4C INPUT FILE FOR THE TEST PROBLEM

```
puo2 mat  1
1 2 -1
  2 0
     094  3.3333338E-01
     008  6.6666662E-01
 -30 1.70000E+01 1.39000E-10
     1.70000E+01 1.50000E+01 1.35000E+01 1.20000E+01 1.00000E+01
     7.79000E+00 6.07000E+00 3.68000E+00 2.86500E+00 2.23200E+00
     1.73800E+00 1.35300E+00 8.23000E-01 5.00000E-01 3.03000E-01
     1.84000E-01 6.76000E-02 2.48000E-02 9.12000E-03 3.35000E-03
     1.23500E-03 4.54000E-04 1.67000E-04 6.14000E-05 2.26000E-05
     8.32000E-06 3.06000E-06 1.13000E-06 4.14000E-07 1.52000E-07
  4
    0942390  2.1215058E+22
    0942400  9.9966255E+20
    0080160  4.4411615E+22
    0080170  1.7816217E+19
  1  100
    0080170  2.6733354E-04
```