Tone's method for resonance self-shielding

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Outline

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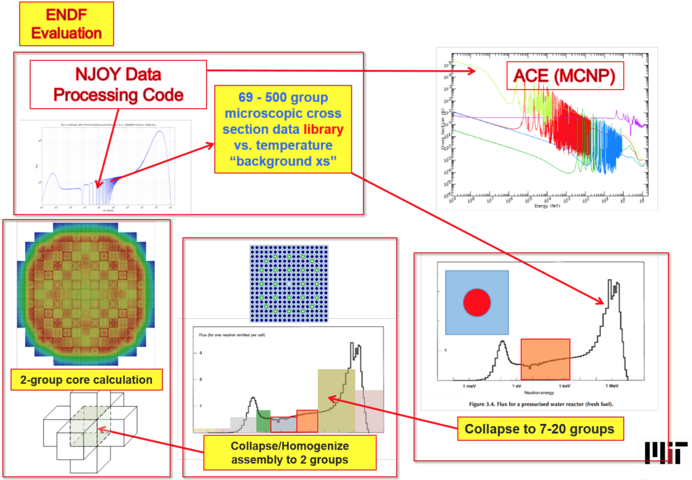
Introduction



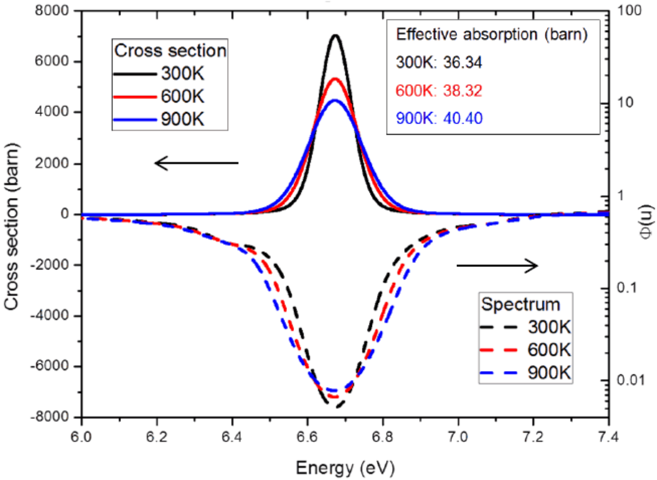


Figure 1: Energy dependent neutron flux versus fuel temperature at 6.67eV resonance of 238U [nuclear-power.net].

Homogeneous Slowing Down

We start with the Boltzmann Equation.

$$\Sigma_t(E)\phi(E) = \int_0^\infty \Sigma_s\left(E' \to E\right)\phi\left(E'\right)\mathrm{d}E' + \frac{\chi(E)}{k_{eff}}\int_0^\infty v\Sigma_f\left(E'\right)\phi\left(E'\right)\mathrm{d}E'$$

Elastic down-scattering is the dominant interaction here, allowing us to eliminate fission term

$$\Sigma_t(E)\phi(E) = \int_0^\infty \Sigma_s\left(E' \to E\right)\phi\left(E'\right)\mathrm{d}E'.$$

Split the macroscopic cross section into its components

$$\left(\sum_k N_k\sigma_{t,k}(E)\right)\phi(E) = \sum_k \int_E^{E/\alpha_k} N_k\sigma_{s,k}\left(E'\right)\phi\left(E'\right)P(E' \to E)\mathrm{d}E'$$

Recall that

$$P(E' \to E)dE' = \frac{1}{(1-\alpha_k)E'}dE',$$

we simplify the scattering term

$$\left(\sum_k N_k \sigma_{t,k}(E)\right)\phi(E) = \sum_k \frac{1}{1-\alpha_k}\int_E^{E/\alpha_k} \frac{1}{E'} N_k \sigma_{s,k}\left(E'\right)\phi\left(E'\right)\mathrm{d}E'$$

Separate resonant nuclide from non-resonant nuclides, and represent non-resonant nuclides using only the potential scattering cross section.

$$\left(N_r\sigma_{t,r}(E) + \sum_{k\neq r} N_k \sigma_{pot,k}\right)\phi(E) = \frac{1}{1-\alpha_r}\int_E^{E/\alpha_r} \frac{N_r\sigma_{s,r}\left(E'\right)\phi\left(E'\right)}{E'}dE' + \sum_{k\neq r}\frac{1}{1-\alpha_k}\int_E^{E/\alpha_k} \frac{N_k\sigma_{pot,k}\phi\left(E'\right)}{E'}dE'$$

Narrow Resonance Approxiamtion A sufficiently thin resonance allows us to approximate that every scattering event will miss the resonance. We thus assume that the scattering kernel is simply equal to the potential scattering cross section σ_{pot}, which is constant in energy.

We now need to simplify the latter integral, which represents **scattering contributions of the non-resonant nuclides**. First, we remove all terms without energy dependence out of the integral, yielding

$$
\begin{aligned}
\text{Non-res scattering} &= \sum_{k \neq r} \frac{1}{1-\alpha_k} \int_E^{E/\alpha_k} \frac{1}{E'} N_k \sigma_{pot,k} \phi\left(E'\right) \mathrm{d}E' \\
&= \sum_{k \neq r} \frac{N_k \sigma_{pot,k}}{1-\alpha_k} \int_E^{E/\alpha_k} \frac{1}{E'} \phi\left(E'\right) \mathrm{d}E' \\
&= \sum_{k \neq r} \frac{N_k \sigma_{pot,k}}{1-\alpha_k} \left(\frac{1}{E} - \frac{\alpha_k}{E}\right) \\
&= \sum_{k \neq r} \frac{N_k \sigma_{pot,k}}{E}
\end{aligned}
$$

$$
\boxed{\sum_{k \neq r} \frac{1}{1-\alpha_k} \int_E^{E/\alpha_k} \frac{1}{E'} N_k \sigma_{pot,k} \phi\left(E'\right) \mathrm{d}E' = \sum_{k \neq r} N_k \sigma_{pot,k} \frac{1}{E}}
$$

We now follow similar steps to simplify the **scattering contributions of the resonant nuclide**. First, we remove all terms without energy dependence out of the integral, yielding

$$
\begin{aligned}
\text{Res scattering} =& \frac{1}{1-\alpha_r}\int_E^{E/\alpha_r}\frac{1}{E'}N_r\sigma_{s,r}\left(E'\right)\phi\left(E'\right)\mathrm{d}E' \\
=& \frac{N_r\sigma_{pot,r}}{1-\alpha_r}\int_E^{E/\alpha_r}\frac{1}{E'}\phi\left(E'\right)\mathrm{d}E' \\
=& \frac{N_r\sigma_{pot,r}}{1-\alpha_r}\left(\frac{1}{E}-\frac{\alpha_r}{E}\right) \\
=& \frac{N_r\sigma_{pot,r}}{E}
\end{aligned}
$$

$$
\boxed{\frac{1}{1-\alpha_r}\int_E^{E/\alpha_r}\frac{1}{E'}N_r\sigma_{pot,r}\phi\left(E'\right)\mathrm{d}E' = N_r\sigma_{pot,r}\frac{1}{E}}
$$

$$\sum_{k \neq r} \frac{1}{1-\alpha_k} \int_E^{E/\alpha_k} \frac{1}{E'} N_k \sigma_{pot,k} \phi\left(E'\right) \mathrm{d}E' = \sum_{k \neq r} N_k \sigma_{pot,k} \frac{1}{E}$$

$$\frac{1}{1-\alpha_r} \int_E^{E/\alpha_r} \frac{1}{E'} N_r \sigma_{pot,r} \phi\left(E'\right) \mathrm{d}E' = N_r \sigma_{pot,r} \frac{1}{E}$$

Putting these together

$$\sum_{k} \frac{1}{1-\alpha_k} \int_E^{E/\alpha_k} \frac{1}{E'} N_k \sigma_{pot,k} \phi\left(E'\right) \mathrm{d}E' = \sum_{k} N_k \sigma_{pot,k} \frac{1}{E}$$

Heterogeneous Slowing Down (Isolated System)

Two region neutron balance:

$$\Sigma_{t,f}(E)\phi_f(E)V_f = P_{f\to f}(E)V_f\int_0^\infty \Sigma_{s,f}\left(E'\to E\right)\phi_f\left(E'\right)dE' + P_{m\to f}(E)V_m\int_0^\infty \Sigma_{s,m}\left(E'\to E\right)\phi_m\left(E'\right)dE'$$

Break apart macroscopic cross sections and substitute in the the probability of energy change via scattering

$$P(E'\to E) = \frac{1}{(1-\alpha)E} \text{ for } \alpha E \le E' \le E,$$

$$\Sigma_{t,f}(E)\phi_f(E)V_f = P_{f\to f}(E)V_f\sum_{k\in f}\int_E^{E/\alpha_k}\frac{N_k\sigma_{s,k}\left(E'\right)\phi_f\left(E'\right)}{\left(1-\alpha_k\right)E'}dE' + P_{m\to f}(E)V_m\sum_{k\in m}\int_E^{E/\alpha_k}\frac{N_k\sigma_{s,k}\left(E'\right)\phi_m\left(E'\right)}{\left(1-\alpha_k\right)E'}dE'.$$

$$\Sigma_{t,f}(E)\phi_f(E)V_f = P_{f\to f}(E)V_f \sum_{k\in f} \int_E^{E/\alpha_k} \frac{N_k\sigma_{s,k}(E')\,\phi_f(E')}{(1-\alpha_k)\,E'} dE'$$
$$+P_{m\to f}(E)V_m \sum_{k\in m} \int_E^{E/\alpha_k} \frac{N_k\sigma_{s,k}(E')\,\phi_m(E')}{(1-\alpha_k)\,E'} dE'.$$

Recall from before

$$\sum_k \frac{1}{1-\alpha_k} \int_E^{E/\alpha_k} \frac{1}{E'} N_k\sigma_{pot,k}\phi(E')\,\mathrm{d}E' = \sum_k N_k\sigma_{pot,k}\frac{1}{E}$$

which helps us simplify the heterogeneous balance equation into

$$\Sigma_{t,f}(E)\phi_f(E)V_f = \frac{1}{E}\Big(P_{f\to f}(E)V_f\Sigma_{pot,f} + P_{m\to f}(E)V_m\Sigma_{pot,m}\Big)$$
$$\phi_f(E) = \frac{P_{f\to f}(E)V_f\Sigma_{pot,f} + P_{m\to f}(E)V_m\Sigma_{pot,m}}{E\Sigma_{t,f}(E)V_f}$$

While this result is derived using a two-region problem, it can be extended to solve for a flux in region $i \in N$, which is dependent on all $j \in N$ regions:

$$\phi_i(E) = \frac{1}{E\Sigma_{t,i(E)} V_i} \sum_j \left(P_{j \to i}(E) V_j \Sigma_{p,j} \right)$$

Remember that we used the NR approximation to get here, which could be a source of error in the lower end of the energy spectrum.

Tone's Method

$$\phi_i(E) = \frac{1}{E\Sigma_{t,i(E)} V_i} \sum_j \left(P_{j\to i}(E) V_j \Sigma_{p,j} \right)$$

Crucial approximation for Tone's Method

$$\frac{P_{j\to i}(E)}{\Sigma_{t,i}(E)} = \alpha_i(E) \frac{P_{j\to i,g}}{\Sigma_{t,i,g}}$$

Allow $P_{j\to i}(E)$ and $\Sigma_{t,i}(E)$ to be constant within a group, but allow a fine energy term α

Fun twist: $\alpha_i(E)$ is only dependent on the region i that our neutrons are going into

$$\phi_i(E) = \frac{\alpha_i(E)}{E\Sigma_{t,i,g} V_i} \sum_j \left(P_{j\to i,g} V_j \Sigma_{p,j} \right)$$

We want more information about $\phi_i(E)$. Doing so requires two additional tools:

1. Reciprocity relation

$$P_{j\to i}(E) V_j \Sigma_{t,j}(E) = P_{i\to j}(E) V_i \Sigma_{t,i}(E)$$

$$P_{i\to j}(E) = \frac{P_{j\to i}(E) V_j \Sigma_{t,j}(E)}{V_i \Sigma_{t,i}(E)}$$

2. Probabilities normalize to 1

$$\sum_j P_{i\to j}(E) = 1$$

Plug reciprocity relation into probabilities requirement

$$\sum_j \left(\frac{P_{j\to i}(E) V_j \Sigma_{t,j}(E)}{V_i \Sigma_{t,i}(E)} \right) = 1$$

$$\sum_j \left(\frac{P_{j\to i}(E) V_j \Sigma_{t,j}(E)}{V_i \Sigma_{t,i}(E)} \right) = 1$$

Plug in the Tone's approximation

$$\frac{P_{j\to i}(E)}{\Sigma_{t,i}(E)} = \alpha_i(E) \frac{P_{j\to i,g}}{\Sigma_{t,i,g}}$$

to yield

$$\frac{\alpha_i(E)}{V_i \Sigma_{t,i,g}} \sum_j \left(P_{j\to i,g} V_j \Sigma_{t,j}(E) \right) = 1$$

$$\alpha_i(E) = \frac{V_i \Sigma_{t,i,g}}{\sum\limits_j \left(P_{j\to i,g} V_j \Sigma_{t,j}(E) \right)}$$

We can now plug this definition of $\alpha_i(E)$ into our earlier equation for $\phi_i(E)$.

$$\phi_i(E) = \frac{\alpha_i(E)}{E\Sigma_{t,i,g}V_i}\sum_j\left(P_{j\to i,g}V_j\Sigma_{p,j}\right)$$

$$\phi_i(E) = \frac{1}{E\Sigma_{t,i,g}V_i}\frac{V_i\Sigma_{t,i,g}}{\sum_j\left(P_{j\to i,g}V_j\Sigma_{t,j}(E)\right)}\sum_j\left(P_{j\to i,g}V_j\Sigma_{p,j}\right)$$

$$\phi_i(E) = \frac{1}{E}\frac{\sum_j\left(P_{j\to i,g}V_j\Sigma_{p,j}\right)}{\sum_j\left(P_{j\to i,g}V_j\Sigma_{t,j}(E)\right)}$$

$$\phi_i(E) \approx \frac{1}{E}\frac{\sum_j\left(P_{j\to i,g}V_j\left(N_{r,j}\sigma_{pot,r} + \sum_{k\neq r}N_{k,j}\sigma_{pot,k}\right)\right)}{\sum_j\left(P_{j\to i,g}V_j\left(N_{r,j}\sigma_{r,t}(E) + \sum_{k\neq r}N_{k,j}\sigma_{pot,k}\right)\right)}$$

$$\phi_i(E) = \frac{1}{E}\frac{\sum_j \left(P_{j\to i,g} V_j N_{r,j} \sigma_{pot,r} + P_{j\to i,g} V_j \sum_{k\neq r} N_{k,j}\sigma_{pot,k} \right)}{\sum_j \left(P_{j\to i,g} V_j N_{r,j} \sigma_{r,t}(E) + P_{j\to i,g} V_j \sum_{k\neq r} N_{k,j}\sigma_{pot,k} \right)}$$

$$\phi_i(E) = \frac{1}{E}\frac{\sigma_{pot,r} \sum_j P_{j\to i,g} V_j N_{r,j} + \sum_j P_{j\to i,g} V_j \sum_{k\neq r} N_{k,j}\sigma_{pot,k}}{\sigma_{r,t}(E) \sum_j P_{j\to i,g} V_j N_{r,j} + \sum_j P_{j\to i,g} V_j \sum_{k\neq r} N_{k,j}\sigma_{pot,k}}$$

$$\phi_i(E) = \frac{1}{E}\frac{\sigma_{pot,r} + \left(\sum_j P_{j\to i,g} V_j \sum_{k\neq r} N_{k,j}\sigma_{pot,k} \Big/ \sum_j P_{j\to i,g} V_j N_{r,j} \right)}{\sigma_{r,t}(E) + \left(\sum_j P_{j\to i,g} V_j \sum_{k\neq r} N_{k,j}\sigma_{pot,k} \Big/ \sum_j P_{j\to i,g} V_j N_{r,j} \right)}$$

$$\phi_i(E) = \frac{1}{E}\frac{\sigma_{pot,r} + \sigma_0}{\sigma_{t,r}(E) + \sigma_0}$$

$$\sigma_0 = \frac{\sum_j \sum_{k \neq r} P_{j \rightarrow i,g} V_j N_{k,j} \sigma_{pot,k}}{\sum_j P_{j \rightarrow i,g} V_j N_{r,j}}$$

Tone's Method

1. Assume initial background cross sections for resonance nuclides, using conventional equivalence methods
2. Evaluate the effective cross sections of resonance nuclides using the conventional equivalence theory
3. Evaluate group-wise collision probability using effective cross sections
4. Update the background cross section using

$$\phi_i(E) = \frac{1}{E}\frac{\sigma_{pot,r} + \sigma_0}{\sigma_{t,r}(E) + \sigma_0}$$

$$\sigma_0 = \frac{\sum_j \sum_{k \neq r} P_{j\to i,g} V_j N_{k,j} \sigma_{pot,k}}{\sum_j P_{j\to i,g} V_j N_{r,j}}$$

5. Repeat until convergence. A few iterations are usually sufficient to obtain the converged result.

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For a heterogeneous system, our background cross section is comprised of a material-component and a geometry-component.

$$\sigma_{0,r} = \sigma_{0,f} + \frac{\Sigma_e}{N_r} = \sum_{k \neq r} \frac{N_k \sigma_{s,k}}{N_r} + \frac{\Sigma_e}{N_r}$$

Note that for Tone's method, the initial estimate for background cross section is not too important since it'll iterate out anyway.

1. Assume initial background cross sections for resonance nuclides, using conventional equivalence methods
2. **Evaluate the effective cross sections of resonance nuclides using the conventional equivalence theory**
3. Evaluate group-wise collision probability using effective cross sections
4. Update the background cross section using

$$\phi_i(E) = \frac{1}{E}\frac{\sigma_{pot,r} + \sigma_0}{\sigma_{t,r}(E) + \sigma_0}$$

$$\sigma_0 = \frac{\sum_j \sum_{k \neq r} P_{j \to i,g} V_j N_{k,j} \sigma_{pot,k}}{\sum_j P_{j \to i,g} V_j N_{r,j}}$$

5. Repeat until convergence. A few iterations are usually sufficient to obtain the converged result.

Use GROUPR to create a table of cross sections vs. dilution for my resonant nuclides.

```
92-u-235                                                                    0 0  0    0
 9.223500+4 2.330248+2          0         10         -1          19228 1451     1
 3.000000+2 0.000000+0         10          0         23          09228 1451     2
 0.000000+0 1.00000+10 1.000000+5 1.000000+4 1.000000+3 8.000000+29228 1451     3
 6.000000+2 4.000000+2 2.000000+2 1.000000+1 1.000000+0 1.000000-59228 1451     4
 5.800000-2 1.400000-1 2.800000-1 6.250000-1 4.000000+0 1.000000+19228 1451     5
 4.000000+1 5.530000+3 8.210000+5 2.000000+7 0.000000+0           9228 1451     6
                                                                  9228 0  0     0
 9.223500+4 0.000000+0          2         10          0         109228 3  1     1
 3.000000+2 0.000000+0          2          1         40          19228 3  1     2
 8.665747+0 8.665739+0 8.039485+0 7.504717+0 5.654376+0 4.177037+09228 3  1     3
 2.196619+0 9.125522-1 1.919842+0 7.246176-1 1.593760+0 5.236503-19228 3  1     4
 1.197523+0 3.140472-1 6.932481-1 1.141632-1 4.150946-2 4.582209-49228 3  1     5
 4.192741-3 4.706571-6 8.532942+3 8.532933+3 7.789918+3 7.125750+39228 3  1     6
 5.325747+3 3.536812+3 2.945042+3 1.407116+3 2.811028+3 1.319564+39228 3  1     7
 2.662381+3 1.226135+3 2.494559+3 1.125278+3 2.300044+3 1.014486+39228 3  1     8
 2.077658+3 8.958832+2 2.065847+3 8.898272+2                      9228 3  1     9
 3.000000+2 0.000000+0          2          1         40          29228 3  1    10
 8.812136-1 8.812136-1 8.782748-1 8.753459-1 8.527006-1 8.251310-19228 3  1    11
 6.612560-1 4.969441-1 6.226094-1 4.408057-1 5.674371-1 3.664993-19228 3  1    12
 4.821898-1 2.651448-1 3.327465-1 1.268095-1 2.615492-2 7.937531-49228 3  1    13
 2.688981-3 8.400117-6 3.346461+2 3.346460+2 3.346191+2 3.345922+29228 3  1    14
 3.343849+2 3.341240+2 3.326362+2 3.306446+2 3.322844+2 3.299481+29228 3  1    15
 3.317829+2 3.289575+2 3.310098+2 3.274361+2 3.296607+2 3.247973+29228 3  1    16
 3.269208+2 3.195095+2 3.267129+2 3.191124+2                      9228 3  1    17
 3.000000+2 0.000000+0          2          1         40          39228 3  1    18
 6.931584-1 6.931584-1 6.915084-1 6.898623-1 6.770048-1 6.612281-19228 3  1    19
 5.596523-1 4.518820-1 5.339482-1 4.113347-1 4.959850-1 3.549360-19228 3  1    20
 4.342445-1 2.720910-1 3.161904-1 1.442878-1 2.791424-2 1.125452-39228 3  1    21
 2.896534-3 1.211911-5 2.386114+2 2.386114+2 2.386107+2 2.386100+29228 3  1    22
 2.386042+2 2.385970+2 2.385518+2 2.384923+2 2.385403+2 2.384694+29228 3  1    23
```

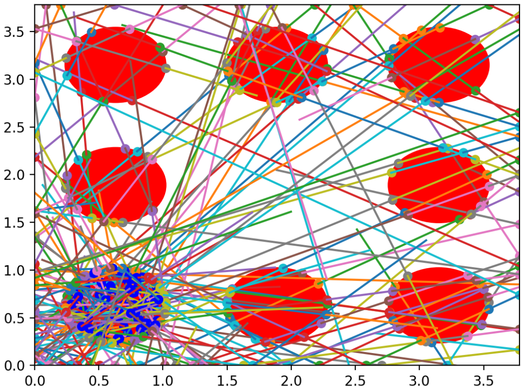
1. Assume initial background cross sections for resonance nuclides, using conventional equivalence methods
2. Evaluate the effective cross sections of resonance nuclides using the conventional equivalence theory
3. **Evaluate group-wise collision probability using effective cross sections**
4. Update the background cross section using

$$\phi_i(E) = \frac{1}{E}\frac{\sigma_{pot,r} + \sigma_0}{\sigma_{t,r}(E) + \sigma_0}$$

$$\sigma_0 = \frac{\sum_j \sum_{k \neq r} P_{j\to i,g} V_j N_{k,j} \sigma_{pot,k}}{\sum_j P_{j\to i,g} V_j N_{r,j}}$$

5. Repeat until convergence. A few iterations are usually sufficient to obtain the converged result.

Created a quick Monte Carlo script that solves for 1 group collision probabilities



Geometry: 3x3 grid, with and without a center hole. Reflective bounds

1. Assume initial background cross sections for resonance nuclides, using conventional equivalence methods
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3. Evaluate group-wise collision probability using effective cross sections
4. **Update the background cross section using**

$$\phi_i(E) = \frac{1}{E}\frac{\sigma_{pot,r} + \sigma_0}{\sigma_{t,r}(E) + \sigma_0}$$

$$\sigma_0 = \frac{\sum_j \sum_{k \neq r} P_{j \to i,g} V_j N_{k,j} \sigma_{pot,k}}{\sum_j P_{j \to i,g} V_j N_{r,j}}$$

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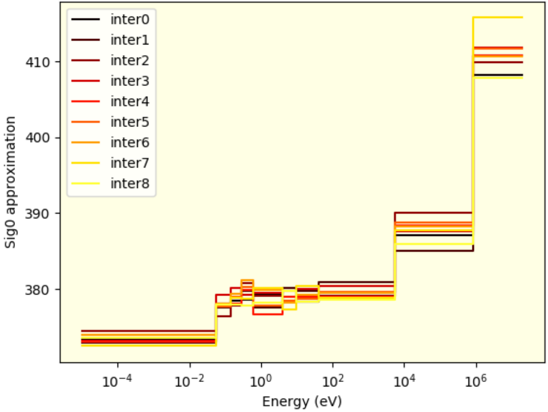
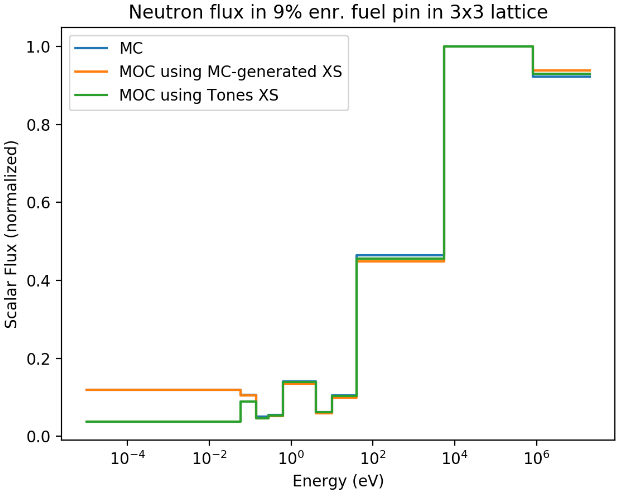
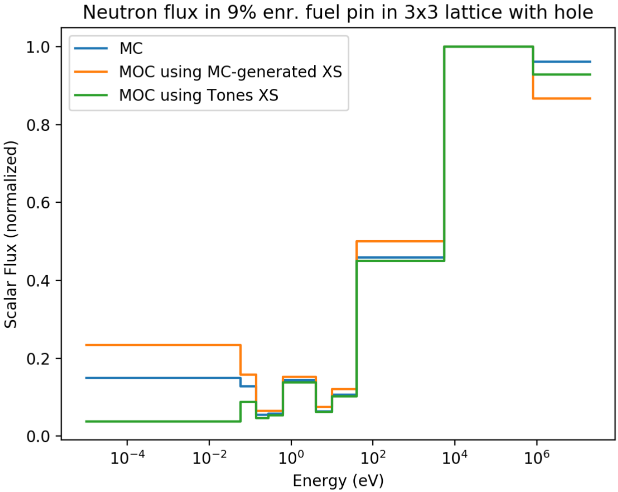
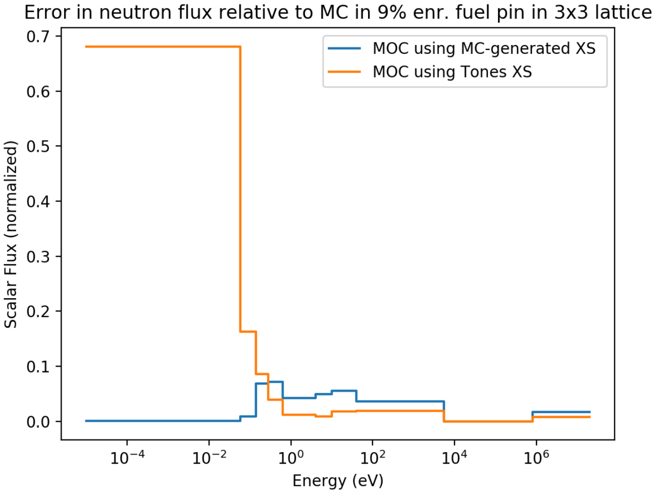
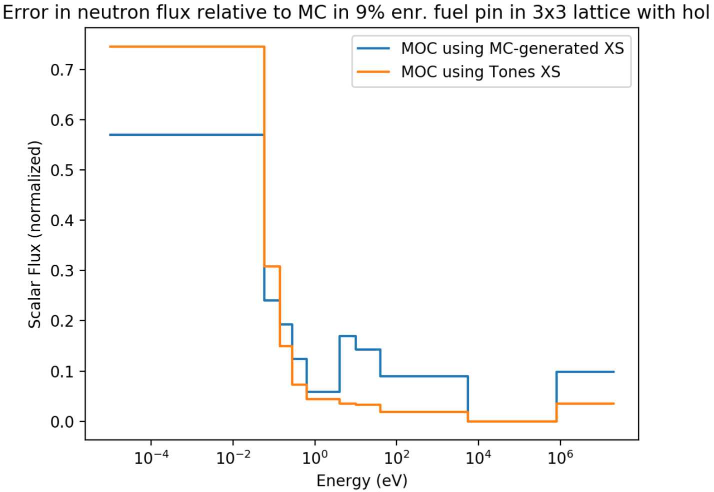


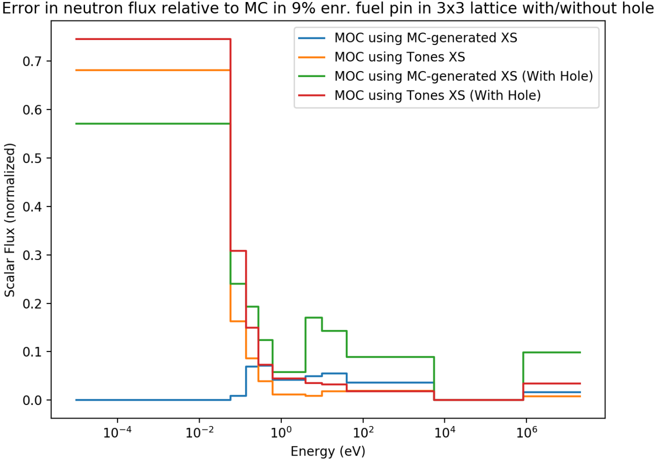
Figure 2: Tone's method evolving background cross section σ_0 across iterations


Neutron flux in 9% enr. fuel pin in 3x3 lattice
MC
MOC using MC-generated XS
MOC using Tones XS
Scalar Flux (normalized)
0.0
0.2
0.4
0.6
0.8
1.0
Energy (eV)
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}


Neutron flux in 9% enr. fuel pin in 3x3 lattice with hole
MC
MOC using MC-generated XS
MOC using Tones XS
Scalar Flux (normalized)
1.0
0.8
0.6
0.4
0.2
0.0
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}
Energy (eV)


Error in neutron flux relative to MC in 9% enr. fuel pin in 3x3 lattice
MOC using MC-generated XS
MOC using Tones XS
Scalar Flux (normalized)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
Energy (eV)
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}


Error in neutron flux relative to MC in 9% enr. fuel pin in 3x3 lattice with hol
MOC using MC-generated XS
MOC using Tones XS
Scalar Flux (normalized)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
10^-4
10^-2
10^0
10^2
10^4
10^6
Energy (eV)


Error in neutron flux relative to MC in 9% enr. fuel pin in 3x3 lattice with/without hole
MOC using MC-generated XS
MOC using Tones XS
MOC using MC-generated XS (With Hole)
MOC using Tones XS (With Hole)
Scalar Flux (normalized)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
Energy (eV)
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}