NE8 Assignment 1: Diffusion

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Regarding this assignment, Dr Cosgrove had informed one of the students via email that it is unnecessary to explain theory in detail, especially when the question does not ask for it. I shall adhere to this recommendation in this report, which will not contain a lot of explanation regarding methodology. However, do note that I have taken the care to thoroughly comment all of my code. These comments should be more than sufficient to understand the method and thought process behind every computation, in case that information is necessary. Feel free to email me for questions about the code, or for additional plots, etc.

1 Macroscopic Constants

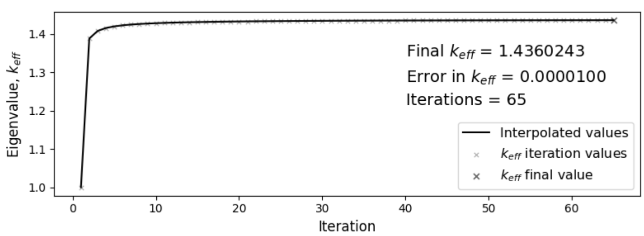
The microscopic constants for each element was given. Since the slab is assumed to be uniform, it is possible to calculate the number density of each element and use that to find the macroscopic constants for each element. The relevant macroscopic constants for the slab was computed from the sum of the macroscopic constants of the elements. The result is as follows:

$$\begin{aligned} D &= 0.52148 \text{ cm} \\ \Sigma_{\mathrm{a}} &= 0.067476 \text{ cm}^{-1} \\ \nu\Sigma_{\mathrm{f}} &= 0.097624 \text{ cm}^{-1} \end{aligned} \tag{1}$$

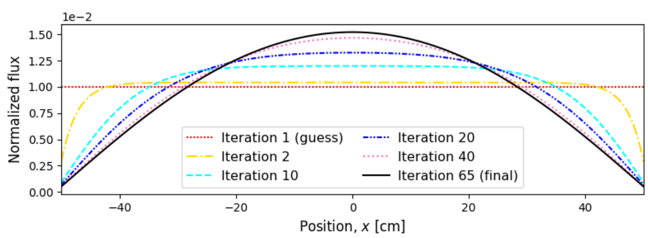
Note that the values shown in Equation 1 are intermittent results that are calculated at the start of program using values that were given in the assignment. The (unrounded) values are stored in variables and used for the calculations below.

2 Solving the Diffusion Equation

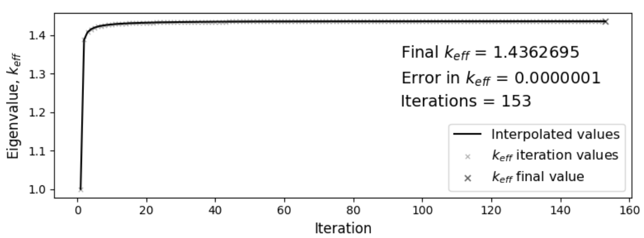
The *finite element approach and source iteration* method for solving the diffusion equation was implemented similarly to the procedure outlined in the `Numerical Methods for Solving the 1D/1E Diffusion Equation` document. From now on, all calculations are done using a mesh resolution of 10 points/cm (1001 points) unless otherwise stated. Results are shown in Figure 1.



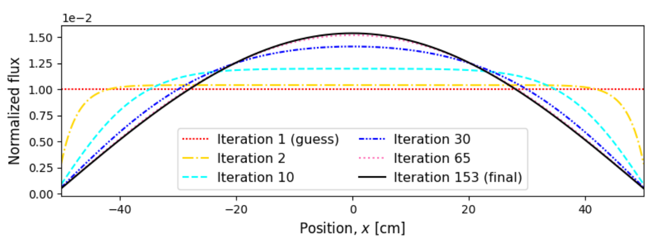
(a) Graph depicting the estimation of the eigenvalue k_{eff} after different iterations using the eigenvalue convergence criterion.



(b) Graph depicting the estimation of the neutron flux ϕ after different iterations using the eigenvalue convergence criterion.



(c) Graph depicting the estimation of the eigenvalue k_{eff} after different iterations using the fission source convergence criterion.



(d) Graph depicting the estimation of the neutron flux ϕ after different iterations using the fission source convergence criterion.

Figure 1: Graphs depicting the eigenvalue convergence and resultant neutron flux distribution of a one-dimensional UO_2 slab in a vacuum. The computation was performed using the *finite element approach and source iteration* method.

The answers to the subquestions are given below.

- **2.1.** *Calculate the criticality eigenvalue (k-eff).*
  - As shown in Figure 1a and Figure 1c, the criticality eigenvalues are:

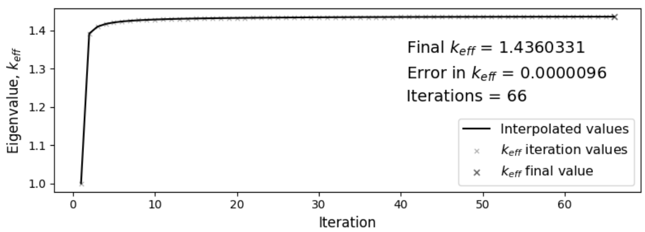
$$\begin{aligned} k_{\text{eff}} &= 1.43602434 \quad \leftarrow \quad k_{\text{eff}} \text{ criterion} \\ k_{\text{eff}} &= 1.43626950 \quad \leftarrow \quad S \text{ criterion} \end{aligned} \tag{2}$$

- **2.2.** *Find the flux distribution within the slab.*
  - The normalized flux distributions are depicted by the solid black lines in Figure 1b and Figure 1d.
- **2.3.** *Find the number of iterations required to satisfy the convergence criteria.*
  - As shown in Figure 1a and Figure 1c, the number of iterations required for the k_{eff} criterion is **65**, while number of iterations required for the S criterion is **153**.
- **2.4.** *Plot the k-eff vs. number of iterations including: the final k-eff value, the final error in k-eff.*
  - The plots are shown in Figure 1a and Figure 1c. NOTE: I was somewhat confused by this question as the error in k_{eff} is only one of the convergence criteria, so I was unsure if I should report the error in S instead for the other one. In case I misinterpreted the question, the error in S is $0.0000095 < 0.000010$.
- **2.5.** *Plot the flux distribution for each iteration on the same graph.*
  - Plots are shown in Figure 1b and Figure 1d. Plotting the sometimes 100+ iterations on the same graph made it way to cluttered, so instead I plotted a few notable ones.
- **2.6.** *Comment on the differences which result from the different convergence criteria.*
  - Looking at Figure 1, the different criteria do not effect the iterations themselves. This makes sense because the calculation of $\phi^{(n+1)}$ does not depend on the convergence criterion. However, the S criterion does take a lot longer to converge. This is why the error in k_{eff} is lower for this criterion. Therefore the S criterion leads to a more accurate result. The difference in k_{eff} between the two criteria is 0.00024516.

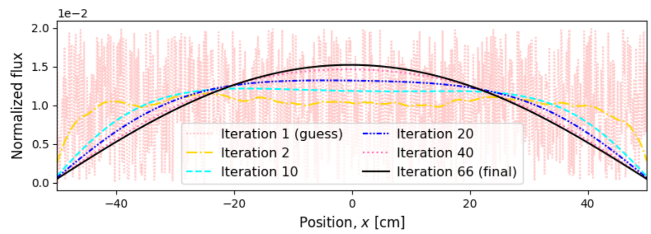
3 Uniform distribution between 0 and 2.

The initial guess was changed to a uniform distribution spanning [0,2]. Plots of the k_{eff} and ϕ convergence of a sample initial guess is depicted in Figure 2. Note that plots for both of the convergence methods are for the same sample guess.

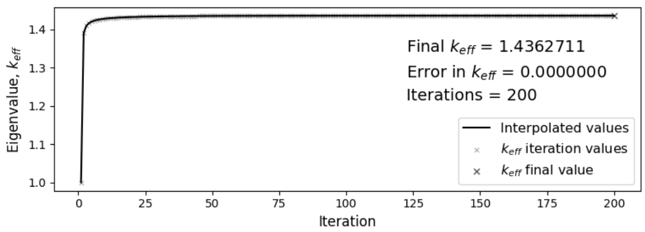
One sample is not enough to comment on the effect of the initial guess on the convergence, so 10000 samples were taken in total. A histogram of the number of iterations is shown in Figure 3. Figure 3a depicts the histogram of the k_{eff} convergence criterion. The random initial guess converges after a mean of $\mu = 65.43 \pm 0.01$ iterations, and has a standard deviation of $\sigma = 1.15$. The histogram clearly shows that the number of iterations follows a normal distribution. Evidently, the initial guess does not greatly effect the convergence. The trivial guess of all ones needed 65 iterations to converge which is slower than slowly 72.6% of guesses.



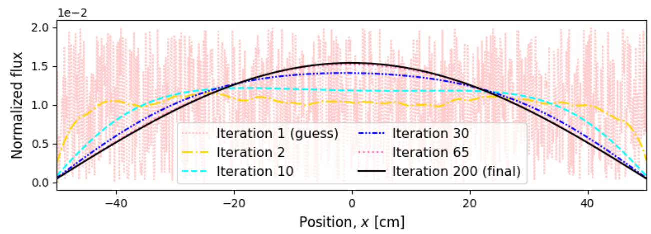
(a) Graph depicting the estimation of the eigenvalue k_{eff} after different iterations using the eigenvalue convergence criterion.



(b) Graph depicting the estimation of the neutron flux ϕ after different iterations using the eigenvalue convergence criterion.

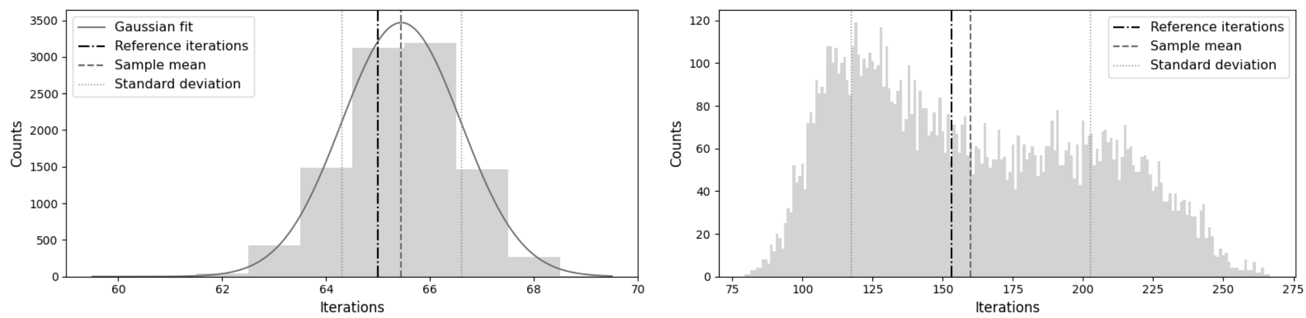


(c) Graph depicting the estimation of the eigenvalue k_{eff} after different iterations using the fission source convergence criterion.



(d) Graph depicting the estimation of the neutron flux ϕ after different iterations using the fission source convergence criterion.

Figure 2: Graphs depicting the eigenvalue convergence and resultant neutron flux distribution calculated from a randomly generated initial neutron flux guess. The initial flux values were taken from a uniform distribution spanning [0,2]. The initial eigenvalue was set to 1. Note that all figures are produced from the same random initial flux guess.



(a) Histogram of the iterations needed for the eigenvalue convergence criterion. The curve depicts a Gaussian generated from the mean and standard deviation.

(b) Histogram of the iterations needed for the fission source convergence criterion.

Figure 3: Histograms of the different numbers of iterations needed before the eigenvalue equation converged. All different samples are all randomly generated initial guesses for the neutron flux, with values taken from a uniform distribution spanning [0,2]. The initial eigenvalue guess was set to 1. The vertical lines indicate various statistical properties of the distributions. Both histograms are generated from the same 10000 random initial flux samples.

Figure 3b depicts the histogram of the S convergence criterion. This time: $\mu = 160.0 \pm 0.4$ and $\sigma = 42.6$. The data appears to have a bimodal distribution. It makes sense that the distribution is much more spread out for this convergence criterion. After all, it is looking at ϕ, which is what starts out randomly. The original guess of all ones converged after 153 iterations, so it converges slower than average.

4 Analytic Solution and Mesh-Size Sensitivity Study

The diffusion equation with a fission source is given by:

$$-\frac{\mathrm{d}}{\mathrm{d}x} D \frac{\mathrm{d}}{\mathrm{d}x} \phi + \left(\Sigma_\mathrm{a} - \frac{\nu\Sigma_\mathrm{f}}{k_\mathrm{eff}}\right)\phi = 0 \tag{3}$$

where k_eff is the unknown eigenvalue that needs to be computed. Define L as:

$$L = \sqrt{\frac{D}{\frac{\nu\Sigma_\mathrm{f}}{k_\mathrm{eff}} - \Sigma_\mathrm{a}}} \tag{4}$$

Substitute Equation 4 in Equation 3 and simplify.

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = -\frac{1}{L^2}\phi \tag{5}$$

Solve by inspection. Note that the setup is symmetric around $x = 0$, so the solution must be even.

$$\phi = A\cos(x/L) \tag{6}$$

By definition, ϕ vanishes at a distance of extrapolation distance z_0 outside the slab.

$$\cos\left(\pm\frac{50 + z_0}{L}\right) = 0 \tag{7}$$

Since $\phi \geqslant 0$, these must be the first roots of the cosine.

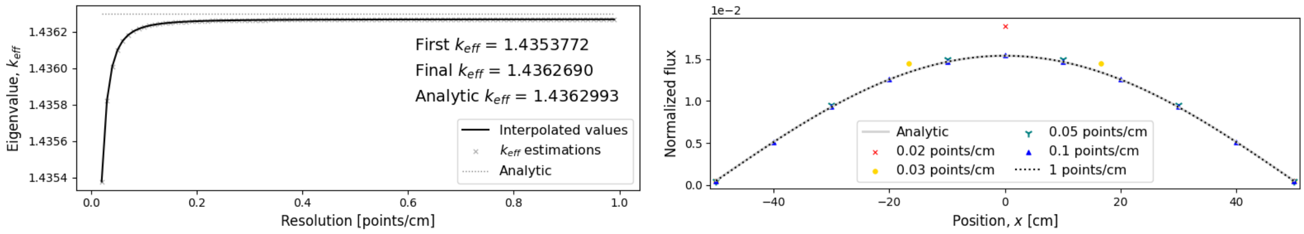
$$\frac{50 + z_0}{L} = \frac{\pi}{2} \tag{8}$$

Solve for L and expand using Equation 4.

$$\sqrt{\frac{D}{\frac{\nu\Sigma_\mathrm{f}}{k_\mathrm{eff}} - \Sigma_\mathrm{a}}} = \frac{2(50 + z_0)}{\pi} \tag{9}$$

Solve for k_eff.

$$k_\mathrm{eff} = \frac{\nu\Sigma_\mathrm{f}}{\frac{D}{4}\left(\frac{\pi}{50 + z_0}\right)^2 + \Sigma_\mathrm{a}} \tag{10}$$



(a) Graph depicting the converged eigenvalue k_{eff} at different resolutions. The dotted horizontal line is the analytic value.

(b) Graph depicting the converged neutron flux ϕ at different resolutions. The solid gray curve is the analytic solution.

Figure 4: Graphs depicting the eigenvalue convergence and resultant neutron flux distribution calculated using different mesh resolutions. Note that a resolution of 0.02 points/cm corresponds to a mesh with 3 points. Both graphs were generated using the source convergence criterion.

The extrapolation distance is given.

$$\begin{aligned} z_0 &= 0.7104\lambda_{\text{tr}} \\ &= 0.7104/\Sigma_{\text{tr}} \end{aligned} \tag{11}$$

So the analytic solution becomes:

$$k_{\text{eff}} = \frac{\nu\Sigma_{\text{f}}}{\frac{D}{4}\left(\frac{\pi}{50+0.7104/\Sigma_{\text{tr}}}\right)^2 + \Sigma_{\text{a}}} \tag{12}$$

The resultant k_{eff} value is:

$$k_{\text{eff}} = 1.43629929 \tag{13}$$

The analytic solution for ϕ is then found using Equation 6, where L is defined according to Equation 4. The answers to the subquestions are given below.

- **4.1.** *Gradually increase the mesh size and repeat the calculation for each new mesh.*
  - A mesh sensitivity study was performed using the S convergence criterion. The resultant graphs are shown in Figure 4. Various numerical values are shown in Table 1.
- **4.2.** *For each mesh size, show the difference in the value of k and the maximum relative difference in the source with respect to the reference.*
  - These values are shown in Table 1. The difference in the value of k_{eff} is shown in the fourth column. The maximum relative difference in ϕ is shown in the seventh column, with the location shown in the eight column. This value was calculated as: $\max|(\phi^{\text{mesh}} - \phi^{\text{analytic}}/\phi^{\text{analytic}})|$.
- **4.3.** *Comment on how the error between the coarse and reference solutions changes with the mesh size.*
  - Looking at Figure 4a, the result of k_{eff} converges extremely quickly, with the value staying pretty constant after 0.2 points/cm. This is also evident in Table 1 where the error stays fairly constant even after the resolution is increased exponentially. Looking at Figure 4b, the flux already becomes virtually indistinguishable from the analytic curve at a resolution of 0.05 points/cm (just 6 points!). In conclusion, although higher resolutions do increase accuracy, this difference is mostly negligible. The resolution of 10 points/cm used for the other exercises is probably overkill.

Table 1: Table showing the eigenvalue convergence at different spatial mesh resolutions, all using the source convergence criterion. The columns respectively depict: the mesh resolution, the resultant eigenvalue, the number of iterations needed, the absolute difference between the calculated and analytic k_{eff}, the maximum absolute difference between the calculated and analytic flux, the location of this error, the maximum relative difference between the calculated and analytic flux compared to the normalized flux, the location of this error. Note that, since the setup is symmetric, the locations are absolute values. Also note that the fluxes were normalized.

Mesh [pts/cm]	k_{eff}	**Iter.**	k_{eff} **diff.**	**Max abs ϕ diff.**	$\lvert x\rvert$ **[cm]**	**Max rel ϕ diff.**	$\lvert x\rvert$ **[cm]**
0.02	1.43537717	31	9.22×10^{-4}	3.58×10^{-3}	0.0	3.58×10^{-3}	0.0
0.03	1.43582148	25	4.78×10^{-4}	1.09×10^{-3}	16.7	1.09×10^{-3}	16.7
0.04	1.43600876	120	2.91×10^{-4}	6.31×10^{-4}	0.0	2.51×10^{-5}	50.0
0.05	1.43610060	129	1.99×10^{-4}	3.52×10^{-4}	10.0	2.81×10^{-5}	50.0
0.10	1.43622669	146	7.26×10^{-5}	6.64×10^{-5}	0.0	3.15×10^{-5}	50.0
1.00	1.43626899	152	3.03×10^{-5}	3.13×10^{-5}	50.0	3.13×10^{-5}	50.0
10.0	1.43626950	153	2.98×10^{-5}	3.11×10^{-5}	50.0	3.11×10^{-5}	50.0
100	1.43626951	153	2.98×10^{-5}	3.11×10^{-5}	50.0	3.11×10^{-5}	50.0

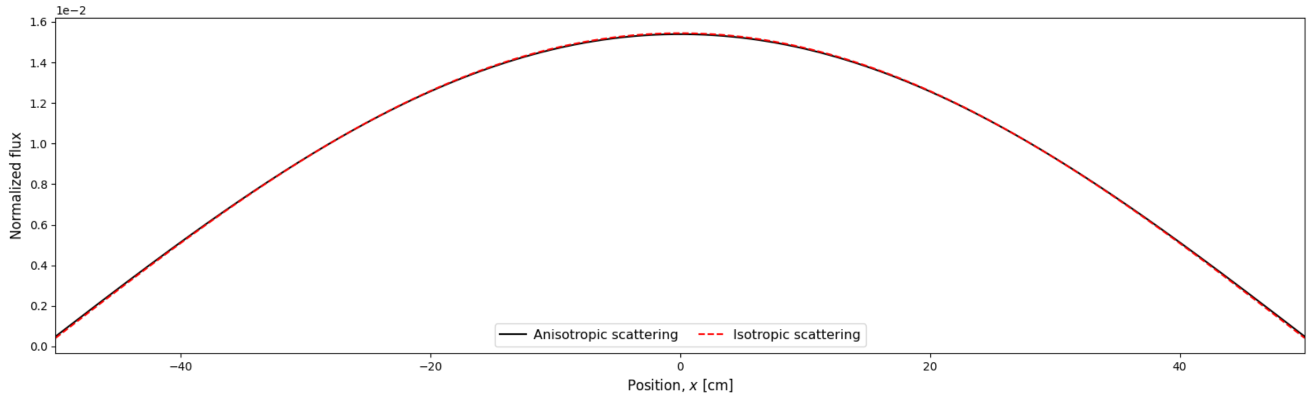


Figure 5: Graph comparing the converged neutron flux ϕ with anisotropic and isotropic scattering. Both curves were generated using the fission source convergence criterion.

5 Effect of Scattering Anisotropy

To determine the effect of anisotropic scattering, the average cosine of scatter $\bar{\mu}$ was set to 0. Using the S convergence criterion resulted in:

$$k_{\text{eff}}^{\text{iso}} = 1.43790507 \tag{14}$$

Compared to the anisotropic value in Equation 2, the isotropic value is higher by 0.00163556. Thus the anisotropy has has a positive impact on k_{eff}.

The normalized ϕ is depicted in Figure 5. Looking closely as this figure, the anisotropic ϕ is slightly more spread out than the isotropic case. This makes sense as a positive value of $\bar{\mu}$ increases the diffusion coefficient.

6 Fixed Fission Power and Fission Products

To start, I want to note that it is unnecessary to normalize ϕ to a fixed fission power at *every* source iteration. The absolute scaling of ϕ has no influence on the source iteration algorithm. However, since the exercise asks for it, I *did* implement it. Still, scaling ϕ just once after the convergence would have been more efficient.

To normalize power, it is first necessary to calculate the areal power P from ϕ. This is done by noting that the nuclear reaction rate is given by the product of the macroscopic cross-section and the neutron flux. Since the energy per fission is a known quantity $Q = 200$ MeV, the total areal power is given by:

$$P = Q\Sigma_{\text{f}} \int \phi(x)\ \mathrm{d}x \tag{15}$$

Obviously, this integral changes to a discrete sum for the computation.

As for fission products (FPs), the equilibrium concentration of Sm-149 is given by:

$$N_{\text{Sm}} = \frac{\gamma_{\text{Sm}}\Sigma_{\text{f}}}{\sigma_{\text{aSm}}} \tag{16}$$

where γ_{Sm} is the cumulative fission yield and σ_{aSm} is the microscopic absorption cross-section. It should be noted that this quantity is independent of ϕ, and can therefore be calculated before the source iteration process. The equilibrium concentration of Xe-135 is given by:

$$N_{\text{Xe}} = \frac{\gamma_{\text{Xe}}\Sigma_{\text{f}}\phi}{\frac{\ln(2)}{t_{1/2}} + \sigma_{\text{aXe}}\phi} \tag{17}$$

where $t_{1/2}$ is the xenon half-life. Unlike Sm-149, this quantity is dependent on flux so it needs to be considered separately. Both Equation 16 and Equation 17 can be found in `NE1 Lecture Notes 10`.

The basic source iteration algorithm used up till now relies on constructing a matrix M^{-1}, and using that to find the eigenpair k_{eff} and ϕ. To recapitulate, M represents the sum of the dispersion and absorption terms in the neutron diffusion equation. In the presence FPs, the absorption term becomes dependent on the Sm-149 and Xe-135 population. However, the Xe-135 population in Equation 17 is dependent on ϕ. This makes M^{-1} also dependent on ϕ, thus making the usual source iteration algorithm impossible.

A solution is to recalculate M^{-1} based on an estimate of ϕ. Runtime analysis of the code using the *LineProfiler* package showed that the calculation of M^{-1} was one of the slowest steps in the source iteration code. Therefore M^{-1} should ideally be recalculated as few times as possible.

The final algorithm works as follows: An initial source iteration of ϕ is performed without any Xe-135 present. This result is used to guess $N_{\text{Xe}}(\phi)$. Then, the $M^{-1}(N_{\text{Xe}})$ matrix is recalculated with Xe-135 present. Now the source iteration is repeated resulting in a new ϕ. This process is repeated until it converges. The following convergence criterion was used:

$$\max\left|\frac{N'_{\text{Xe}} - N_{\text{Xe}}}{N_{\text{Xe}}} < 0.00001\right| \tag{18}$$

where N'_{Xe} denotes a newly calculated Xe-135 concentration. The result is shown in Figure 6. The subquestions are answered below.

- **6.1.** *Plot the spatial distribution of fission products' concentrations*
  - The concentration of FPs is plotted in Figure 6b. The equilibrium concentration for Sm-149 is:

    $$N_{\text{Sm}} = 6.12859022 \cdot 10^{16}\ \text{cm}^{-3} \tag{19}$$

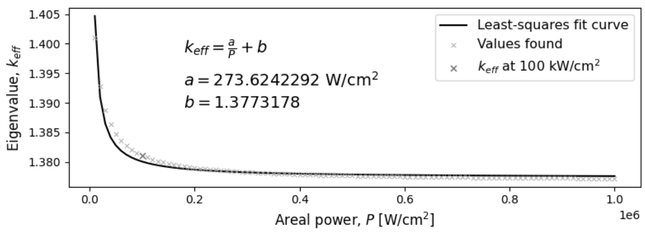
    The maximum, minimum and average concentration of Xe-135 are:

    $$\begin{aligned} \max\ N_{\text{Xe}} &= 1.05217530 \cdot 10^{16}\ \text{cm}^{-3} \\ \min\ N_{\text{Xe}} &= 3.57077620 \cdot 10^{15}\ \text{cm}^{-3} \\ \overline{N_{\text{Xe}}} &= 9.71277146 \cdot 10^{15}\ \text{cm}^{-3} \end{aligned} \tag{20}$$

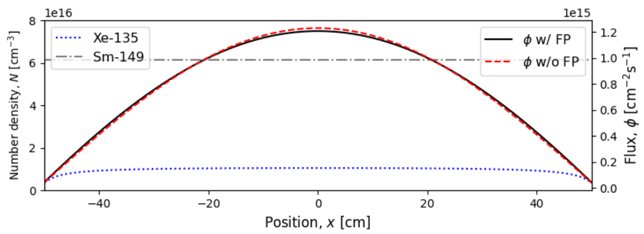
- **6.2.** *Compare the poison equilibrium flux distribution and criticality eigenvalue with those obtained in sections 2.1 and 2.2. Comment on the results.*
  - The resultant k_{eff} is given by:

    $$k_{\text{eff}} = 1.38108731 \tag{21}$$

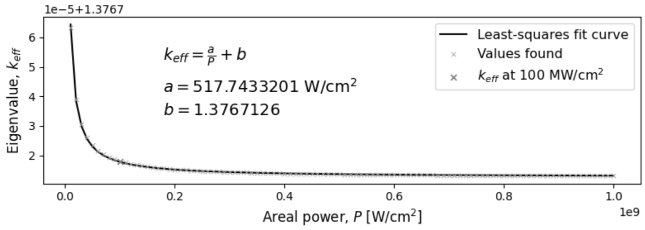
    which is lower than the original value in Equation 2. This makes sense as SM-149 and Xe-135 have high absorption cross-sections and therefore reduce the number of neutrons who make it to the next generation. Looking at Figure 6b, the neutron flux appears to be lower in the center compared to the original case. This makes sense as there is more Xe-135 present in the center.
- **6.3.** *Vary the reactor power production over a wide range of values and comment on the effect on criticality.*
  - The equilibrium power was varied from 10-1000 kW/cm^2. The result is shown in Figure 6a. The relationship appeared to be inversely proportional. However, plotting the least-squares curve shows that it does not perfectly follow such a relationship. Power was varied again but from 10-1000 MW/cm^{-2}. Interestingly, Figure 6c shows that the inverse proportional relationship holds up much better at high P. Looking at Figure 6d, the Xe-135 concentration becomes almost constant, which makes sense looking at Equation 17. The ϕ terms dominate and cancel. As a result, ϕ also approaches the FP free curve.



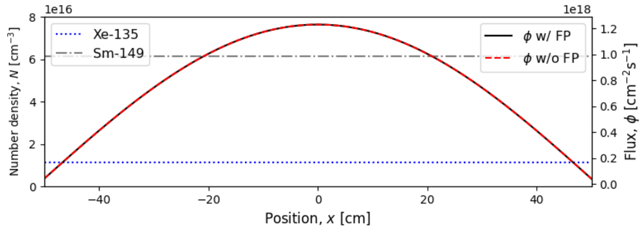
(a) Graph depicting the correlation between the value of k_{eff} and the areal power P. The crosses represent individual data points. The solid line is the least-squares curve of an inversely proportional relation.



(b) Graph depicting the converged neutron flux and equilibrium concentration of fission products throughout the slab. The red line represents the flux obtained without fission products present. This graph is for an areal power of $P = 100$kW/cm^2.



(c) Graph depicting the correlation between the value of k_{eff} and the areal power P. The crosses represent individual data points. The solid line is the least-squares curve of an inversely proportional relation.



(d) Graph depicting the converged neutron flux and equilibrium concentration of fission products throughout the slab. The red line represents the flux obtained without fission products present. This graph is for an areal power of $P = 100$MW/cm^2.

Figure 6: Graphs depicting the eigenvalue convergence and resultant neutron flux distribution with fission products included and flux normalized to a specific areal power. (a) and (b) depict the kW/cm^2 range, while (c) and (d) depict the MW/cm^2 range. All computations were done using the fission source convergence criterion.