The Neutron Diffusion Equation

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Abstract

In this report, the neutron diffusion equation is solved numerically and analytically for homogeneous Dirichlet boundary conditions and numerically for Neumann boundary conditions and a mix of homogeneous Dirichlet and Neumann. When assuming all constants were equal to 1, for Dirichlet and

mixed boundary conditions this lead to critical lengths of $L = \pi$, 0.79 respectively, while Neumann boundary conditions had no critical length. Additionally, a tamper was modeled by extending the boundary on both sides with a region in which the heat equation is obeyed; leading to critical lengths of 1.72, 0.88 and 0.60 for extension factors $\alpha =$, 2 6 and 12 respectively.

1 INTRODUCTION

On 13th August 1942, the United States began a top secret project to develop the world's first atomic bomb, culminating in the creation of the largest bombs ever used in warfare. This report studies the equation that describes the flux of neutrons, the neutron diffusion equation. In 1D, this is given by

$$\frac{\partial n(x,t)}{\partial t} = D\frac{\partial^2 n(x,t)}{\partial x^2} + Cn(x,t) \tag{1}$$

where D and C are constants that depend on the element. For $^{235}_{92}U$, D and C are approximately equal to 1×10^5 and 1×10^8 respectively. For all calculations done in this report these will be kept at 1, however, for all derivations D and C are kept as unknown constants for generality

Three boundary conditions are studied: one where the boundaries are set to 0 (homogeneous Dirichlet), where one boundary is set to 0 and the other has the spatial derivative set to 0, and one where both boundaries have spatial derivatives equal to 0 (homogeneous Neumann):

$$n(-\frac{L}{2}, t) = n(\frac{L}{2}, t) = 0 \tag{2}$$

$$\frac{\partial n(-\frac{L}{2}, t)}{\partial x} = n(\frac{L}{2}, t) = 0 \tag{3}$$

$$\frac{\partial n(-\frac{L}{2}, t)}{\partial x} = \frac{\partial n(\frac{L}{2}, t)}{\partial x} = 0 \tag{4}$$

Each with the initial condition of a Dirac delta at $x = 0$

$$u(x, 0) = \delta(x) \tag{5}$$

For the numerical solutions, this is approximated as $\frac{1}{\Delta x}$.

Also considered is the addition of a tamper at the boundaries, modeled as regions where $C = 0$. The range is extended to $-\frac{\alpha L}{2} \leq x \leq \frac{\alpha L}{2}$ and regions where $x \leq |\frac{L}{2}|$ C is non zero. This was done for the factors $\alpha = 2, 6$ and 12.

The goal of this report is to determine the critical lengths of the system. This is the minimum length in which after some time, the system will always be increasing, i.e. the system reaches a steady state.

2 ANALYTICAL

2.1 SEPARATION OF VARIABLES

One way to solve this is to assume the solution has the form:

$$n(x,t) = \xi(x)\eta(t). \tag{6}$$

Subbing this into eq.(1) and dividing by $n(x,t)$ gives

$$\frac{1}{D\eta}\frac{\partial\eta}{\partial t} - C = \frac{1}{\xi}\frac{\partial^2\xi}{\partial x^2} \tag{7}$$

As x and t are independent of each other, and as the LHS only depends on t and the RHS only depends on x, both sides must be constant (if the LHS did change with t, then the RHS would have to too, contradicting the fact x is independent of t). This can be written in the form of two ODEs

$$-\lambda = \frac{1}{D\eta}\frac{\partial\eta}{\partial t} - C \tag{8}$$

$$-\lambda = \frac{1}{\xi}\frac{\partial^2\xi}{\partial x^2} \tag{9}$$

Starting with Eq. (8), the constants are taken to one side and both sides and integrated w.r.t time

$$\int \frac{1}{\eta}\frac{\partial\eta}{\partial t}dt = \int(-D\lambda + C)dt \tag{10}$$

$$\ln\eta = (-D\lambda + C)t + \beta \tag{11}$$

where φ is a constant of integration. Rearranging and setting $\gamma = e^{\beta}$ give the time dependence of $u(x,t)$

$$\eta(t) = \gamma e^{(-D\lambda+C)t} \tag{12}$$

Now returning to Eq. (9), assuming real values and positive $\lambda = +\omega^2$, Eq. (14) gives

$$\frac{\partial^2\xi}{\partial x^2} + \omega^2\xi = 0 \tag{13}$$

This has the general solution

$$\xi(x) = A\cos(\sqrt{\lambda}x) + B\sin(\sqrt{\lambda}x) \tag{14}$$

Subbing the boundary conditions in, Eq.(14) becomes

$$\xi(x) = A\cos(\frac{\omega L}{2}) + B\sin(\frac{\omega L}{2}) \tag{15}$$

$$\xi(x) = A\cos(\frac{\omega L}{2}) - B\sin(\frac{\omega L}{2}) \tag{16}$$

Subtracting Eq.(18) from Eq.(15) gives

$$\xi(x) = 2B \sin(\frac{\omega L}{2}) \tag{17}$$

And so $B = 0$. Adding the equations gives:

$$\xi(x) = 2A \cos(\frac{\omega L}{2}) \tag{18}$$

$A = 0$ would be trivial, so take $\cos(\frac{\omega L}{2}) = 0$. This is true when $\frac{\omega L}{2} = \pi(n - 1/2)$ for $n = 1, 2, ...$ and rearranging gives $\omega = \frac{(2n-1)\pi}{L}$. Subbing $\xi(x)$ and $\lambda = \omega^2$ into Eq.(6) gives

$$u(x,t) = \sum_{n=1}^{\infty} B_{2n-1} \cos(\frac{(2n-1)\pi x}{L}) \exp((C - D(\frac{(2n-1)\pi}{L})^2)t) \tag{19}$$

Now all that is needed are the B_{2n-1}. These are found by applying the initial condition, multiplying both sides by $\cos(\frac{m\pi x}{L})$ and integrating w.r.t. x

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} \cos(\frac{m\pi x}{L})\delta(x)dx = \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos(\frac{m\pi x}{L}) \sum_{n=1}^{\infty} B_{2n-1} \cos(\frac{(2n-1)\pi x}{L}) \tag{20}$$

On the LHS, $\delta(x)$ cancels out all terms other than $\cos(0)$, and hence the LHS is equal to 1. On the RHS, due to the orthogonality of cosine:

$$\int_0^L \cos(\frac{mx}{2})\cos(\frac{nx}{2}) = \begin{cases} L & m = n = 0 \\ \frac{L}{2} & m = n \\ 0 & m \neq n \end{cases} \tag{21}$$

The only term to survive is when $m = 2n - 1$, hence leaving

$$B_m = \frac{2}{L} \tag{22}$$

Therefore, the solution to the 1D neutron diffusion equation for homogeneous Dirichlet boundary conditions is

$$u(x,t) = \frac{2}{L} \sum_{n=1}^{\infty} \cos(\frac{(2n-1)\pi x}{L}) \exp((C - D(\frac{(2n-1)\pi}{L})^2)t) \tag{23}$$

The critical length is the minimum length in which the solution will have increasing solutions with time. This must be when the coefficient of t in the exponential above is equal to 0, since negative power exponentials decay and positive exponentially increase. Therefore

$$C = D(\frac{(2n-1)\pi}{L})^2$$

$$L = (2n-1)\pi\sqrt{\frac{D}{C}}$$

$$L_{crit} = \pi\sqrt{\frac{D}{C}} \tag{24}$$

Where $n = 1$ since this gives the smallest possible value of L

3 Numerical

3.1 Finite Difference

To solve the PDE numerically, x, t and u have to be discretised - this can be represented as a matrix with elements n_{ij}, where i is the ith step in space and j is the jth step in time. One way to do this is by expressing the derivatives in their finite difference form. From there, a formula can be derived to move a state of the system forward in time.
The first derivative of t is given by the 2 point forward difference:

$$n_t(i,j) = \frac{n(i,j+1) - n(i,j)}{\Delta t} \tag{25}$$

The second derivative of x is given by a 3 point central difference:

$$n_{xx}(i,j) = \frac{n(i+1,j) - 2n(i,j) + n(i-1,j)}{(\Delta x)^2} \tag{26}$$

These can then be subbed into Eq.(1).

$$\frac{n(i,j+1) - n(i,j)}{\Delta t} = D\frac{n(i+1,j) - 2n(i,j) + n(i-1,j)}{(\Delta x)^2} + Cn(i,j) \tag{27}$$

Looking at the two derivatives, only the $n(i,j+1)$ term changes with time. So, by re-arranging Eq.(27) for this term, an equation that steps the system forward one step in time is found:

$$n(i,j+1) = \alpha(n(i+1,j) - 2n(i,j) + n(i-1,j)) + (C\Delta t + 1)n(i,j) \tag{28}$$

where $\alpha = \frac{D\Delta t}{(\Delta x)^2}$. Therefore, the value of n only depends on the 3 values from the previous time step.

$$\begin{pmatrix} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & u_{i-1,j} & u_{i,j} & u_{i+1,j} & \cdots \\ \cdots & \cdots & u_{i,j+1} & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

The n matrix begins as a matrix filled with 0s. The initial condition is made by setting the middle element of the first row of n to be $\frac{1}{\Delta x}$. To satisfy Eq.(2) are set by simply not calculating n_{ij} at the boundary. Neumann boundary conditions are handled by rearranging the finite difference formula for the first derivatives. Using forward difference for the first element in the row:

$$\frac{n(i+1,j) - n(i,j)}{\Delta x} = 0 \tag{29}$$

$$n(i+1,j) - n(i,j) = 0 \tag{30}$$

$$n(i+1,j) = n(i,j) \tag{31}$$

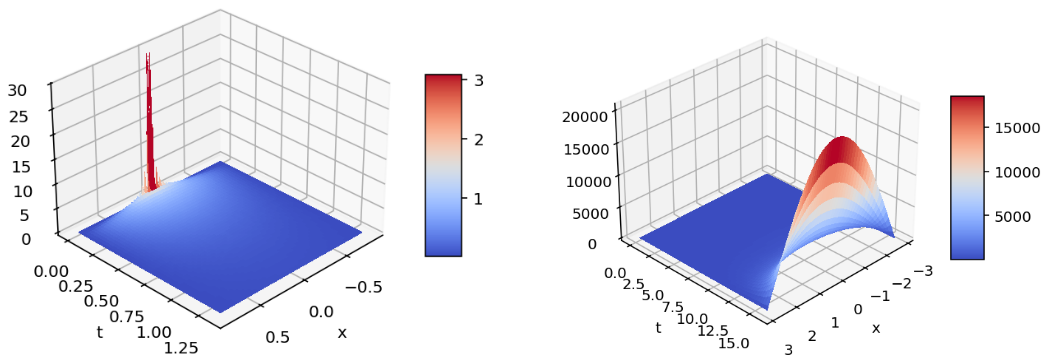
Therefore, the first element is equal to the second. Backwards difference is needed for the last element, since there is no $i + 1$th term:

$$\begin{aligned}\frac{n(i,j) - n(i-1,j)}{\Delta x} &= 0\\ n(i,j) - n(i-1,j) &= 0\\ n(i,j) &= n(i-1,j)\end{aligned}$$

Therefore, the last element is equal to the second last.

4 RESULTS

4.1 DIRICHLET BOUNDARY CONDITIONS



(a) Length = 1.64

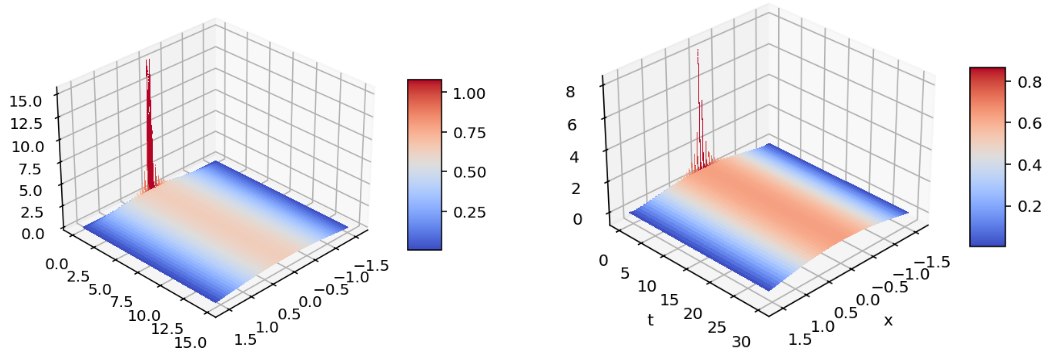
(b) length = 5.64

Figure 1: 3D plots of the numerical solution to the neutron diffusion equation for (a) below the critical length and (b) above the critical length with the boundary conditions $n(-\frac{L}{2}, t) = n(\frac{L}{2}, t) = 0$

Fig.1 shows the numerical solution for below (Fig.1a) and above (Fig.1b) the critical length. The solutions grow exponentially faster as length increases; this can be understood physically as the neutrons having more time to gain energy before leaving the system. The critical length was taken to be the length in which the mean of a time step remains constant, which was found by fitting a straight line to the mean of the last 10% of time steps and determining what length the gradient is zero. Using the bisection method, a critical length of π was found, which agrees with Eq.(24) when $D = C = 1$. The 3D plots for the numerical and analytical solution $L = \pi$ is shown in Fig.2.

4.2 NEUMANN BOUNDARY CONDITIONS

Fig.3 shows a diverging solution for the boundary conditions in Eq.(4). When the bisection method was applied to this system, the gradient was positive for all L tested.



(a) Finite Difference

(b) Separation of Variables

Figure 2: 3D plots of solutions to the neutron diffusion equation for (a) finite difference and (b) Separation of Variables with the boundary conditions $n(-\frac{L}{2}, t) = n(\frac{L}{2}, t) = 0$ at the critical length

This suggests there is no critical length for such a system, however, since no analytical solution was found this cannot be confirmed.

4.3 Mix of Boundary Conditions

Fig.4 shows the numerical solutions for (a) below and (b) above the critical length. The effect of the mixed boundaries is that the solution rises significantly more on the side of the derivative boundary. The critical length is much lower than for Dirichlet boundaries, with $L = 0.79$.

4.4 Tamper

Fig.6 shows 3D plots for different tamper sizes. For $\alpha = 2, 6$ and 12, critical lengths of $L = 1.72, 0.88$ and 0.60 were found using bisection. In each of the tamper sizes, the solution was much more concentrated in the region where $C \neq 0$. Fig.6d shows how critical length varies with α. As α increases, the critical length exponentially decays.

5 Conclusion

This report showed an analytical and a numerical solution to the 1D neutron diffusion equation for 4 sets of boundary conditions. Increasing L causes an increase in the magnitude of the solution. The critical length depends on the boundary conditions, with Dirichlet boundary conditions increasing the critical length and Neumann decreasing it. As the size of a tamper increases, the critical length falls exponentially. Future work should include an analytical solution to the system with Neumann boundary conditions to test if it increases with time regardless of L.

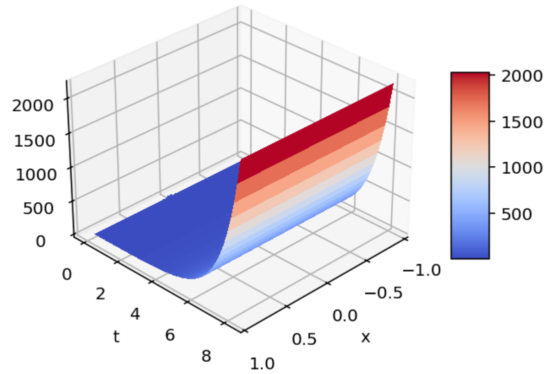
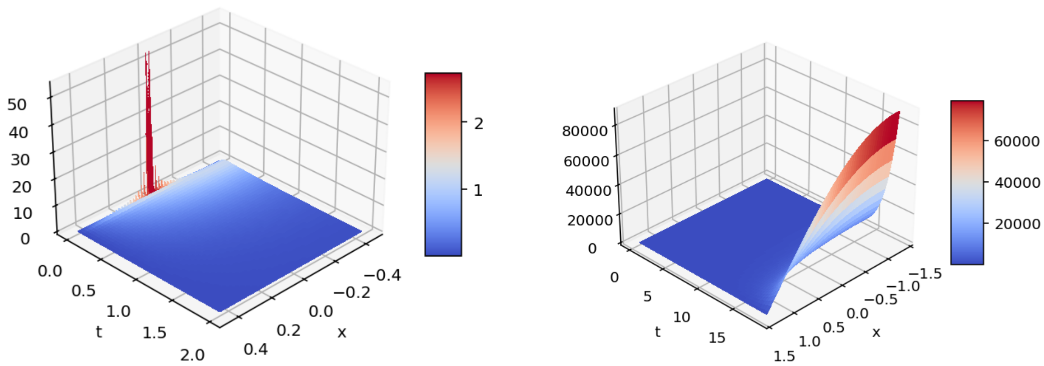


Figure 3: 3D plot of solution to the neutron diffusion equation for homogeneous Neumann boundary conditions



(a) Length = 0.89

(b) length = 2.7

Figure 4: 3D plots of the numerical solution to the neutron diffusion equation for (a) below the critical length and (b) above the critical length with the boundary conditions $\frac{\partial n(-\frac{L}{2},t)}{\partial x} = n(\frac{L}{2},t) = 0$

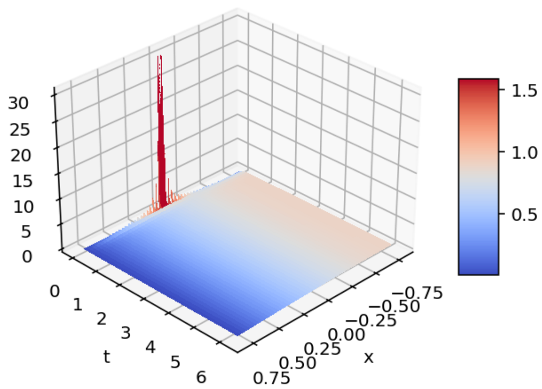
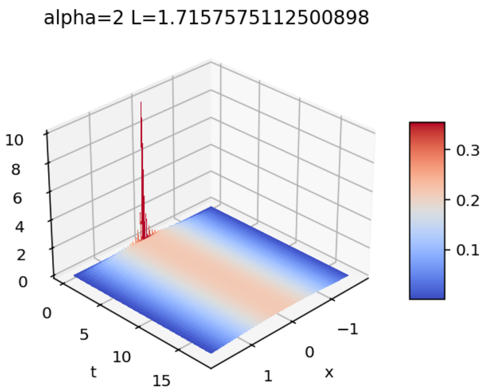
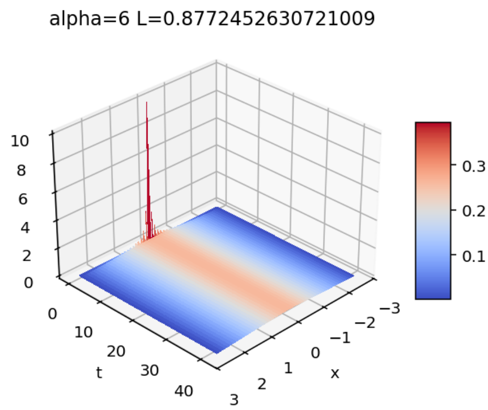


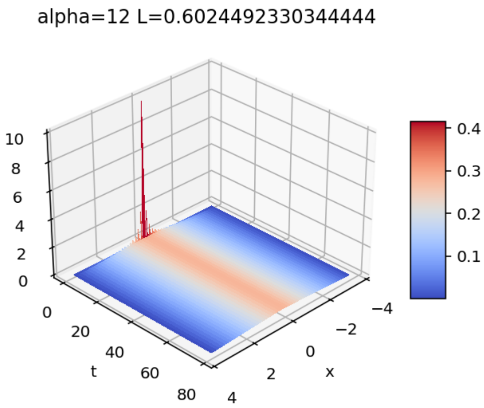
Figure 5: 3D plots of the numerical solution to the neutron diffusion equation at the critical length for one boundary set at 0 and the other with spatial derivative set to zero



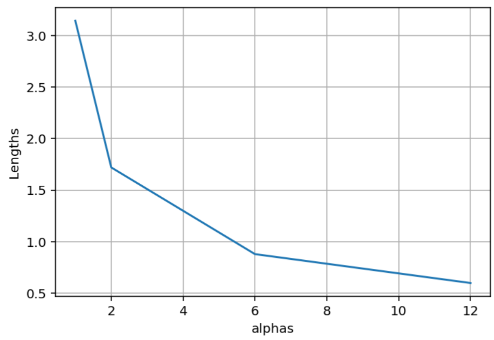
(a) $\alpha = 2$



(b) $\alpha = 6$



(c) $\alpha = 12$



(d) Graph of critical length against α

Figure 6: 3D plots of the numerical solution to the neutron diffusion equation at the critical length and boundary conditions $n(-\frac{L}{2}, t) = n(\frac{L}{2}, t) = 0$ and (a) $\alpha = 2$, (b) $\alpha = 6$, (c) $\alpha = 12$ and (d) plot showing how increasing α causes an exponential decay in the critical length