THE DRIFT-DIFFUSION LIMIT OF THERMAL NEUTRONS:

Theoretical and Numerical Results

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New Approach for Modeling Thermal Neutrons

- Our underlying model for thermal neutrons is derived through an asymptotic analysis of the 1-D energy-dependent transport equation
- In this asymptotic analysis:
  - σ_a is assumed to be small → Order ϵ
  - Q is assumed to be small → Order ϵ
  - σ_s is assumed to be large → Order $1/\epsilon$
- This asymptotic analysis leads to a *drift-diffusion equation*
  - which is believed to handle large temperature gradients

Numerical Comparison

- The second half of this presentation will show numerical comparisons between the drift-diffusion model and MCNP6
  - This will demonstrate how closely our analytical model can predict the spatial-flux distribution in large moderator with a temperature gradient
- The first test problem for our analytical model is to predict the flux in a graphite slab with a *linear* temperature gradient
- The second test problem is to predict the flux in a graphite slab with a *quadratic* temperature gradient

Asymptotic Analysis of Transport Eq.

- We start with the 1-D energy-dependent transport equation

$$\mu\frac{\partial\psi}{\partial x}+(\sigma_{\mathrm{s}}(E)+\sigma_{\mathrm{a}}(E))\,\psi(x,\mu,E)=\int_0^\infty \mathrm{d}E'\int_{4\pi}\mathrm{d}\Omega'\sigma_{\mathrm{s}}(E')f(E'\to E,\mu_0)\psi(\Omega',E')+\frac{Q}{2}$$

- We write the angular flux as a power series

$$\psi\to\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\ldots$$

- Make the following assumptions: σ_a is small → Order ϵ
  Q is small → Order ϵ
  σ_s is large → Order $1/\epsilon$

$$\mu\frac{\partial}{\partial x}(\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\ldots)+\left(\frac{\sigma_{\mathrm{s}}(E)}{\epsilon}+\epsilon\sigma_{\mathrm{a}}(E)\right)(\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\ldots)=$$

$$\int_0^\infty \mathrm{d}E'\int_{4\pi}\mathrm{d}\Omega'\frac{\sigma_{\mathrm{s}}(E')}{\epsilon}f(E'\to E,\mu_0)(\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\ldots)+\epsilon\frac{Q}{2}$$

Splitting up the Transport Eq. by Order

- If ϵ is very small → the terms of order $1/\epsilon$ are only effected by other terms of order $1/\epsilon$
  - By canceling out all other terms in the equation we're left with a $1/\epsilon$ order equation
- The same can be done for terms of order 1 and terms of order ϵ
- Thus the equation

$$\mu\frac{\partial}{\partial x}(\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\dots)+\left(\frac{\sigma_{\mathrm{s}}(E)}{\epsilon}+\epsilon\sigma_{\mathrm{a}}(E)\right)(\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\dots)=$$
$$\int_0^\infty \mathrm{d}E'\int_{4\pi}\mathrm{d}\Omega'\frac{\sigma_{\mathrm{s}}(E')}{\epsilon}f(E'\to E,\mu_0)(\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\dots)+\epsilon\frac{Q}{2}$$

can be used to make 3 separate equations: one with terms of order $1/\epsilon$, another of order 1, and another of order ϵ

Equation of Order $1/\epsilon$

$$\mu\frac{\partial}{\partial x}(\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\ldots)+\left(\frac{\sigma_\mathrm{s}(E)}{\epsilon}+\epsilon\sigma_\mathrm{a}(E)\right)(\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\ldots)=$$
$$\int_0^\infty \mathrm{d}E'\int_{4\pi}\mathrm{d}\Omega'\frac{\sigma_\mathrm{s}(E')}{\epsilon}f(E'\to E,\mu_0)(\psi^{(0)}+\epsilon\psi^{(1)}+\epsilon^2\psi^{(2)}+\ldots)+\epsilon\frac{Q}{2}$$

- After eliminating smaller terms, the $1/\epsilon$ order equation is

$$\frac{\sigma_\mathrm{s}(E)}{\epsilon}\psi^{(0)}(x,\mu,E)=\int_0^\infty \mathrm{d}E'\int_{4\pi}\mathrm{d}\Omega'\frac{\sigma_\mathrm{s}(E')}{\epsilon}f(E'\to E,\mu_0)\psi^{(0)}(x,\Omega',E')$$

- By noticing that the equation above is for an infinite medium with no source and no absorption, we know the solution will be a Maxwellian

$$\psi^{(0)}(x,\mu,E)=\frac{\bar{\phi}^{(0)}(x)}{2}M(E,T(x))$$

Equation of Order 1

- After eliminating all other terms, the equation of order 1 is

$$\mu\frac{\partial\psi^{(0)}}{\partial x}+\sigma_{\rm s}(E)\psi^{(1)}(x,\mu,E)=\int_0^\infty {\rm d}E'\int_{4\pi}{\rm d}\Omega'\sigma_{\rm s}(E')f(E'\to E,\mu_0)\psi^{(1)}(\Omega',E')$$

- After multiplying both sides by μ and integrating from -1 to 1 we arrive at

$$\frac{1}{3}\frac{d\phi^{(0)}(x,E)}{dx}+\sigma_{\rm s}(E)[1-\mathcal{S}_1]J^{(1)}(x,E)=0$$

where S_1 is a group-to-group scattering operator for the first Legendre moment

$$S_l\phi(E)=\frac{1}{\sigma_{\rm s}(E)}\int_0^\infty {\rm d}E'\sigma_{\rm s}(E')f_l(E'\to E)\phi(E')$$

Equation of Order ϵ

- After eliminating all other terms, the equation of order ϵ is

$$\epsilon\mu\frac{\partial\psi^{(1)}}{\partial x}+\epsilon\sigma_{\mathrm{s}}(E)\psi^{(2)}(x,\mu,E)+\epsilon\sigma_{\mathrm{a}}(E)\psi^{(0)}(x,\mu,E)=$$

$$\epsilon\frac{Q}{2}+\int_0^\infty \mathrm{d}E'\int_{4\pi}\mathrm{d}\Omega'\,\epsilon\sigma_{\mathrm{s}}(E')f(E'\to E,\mu_0)\psi^{(2)}(x,\Omega',E')$$

- After multiplying both sides by μ and integrating from -1 to 1, and using the property that

$$\int_0^\infty dE\int_{-1}^1 d\mu_0\,f(E'\to E,\mu_0)=1$$

it can be shown that

$$\frac{d\bar{J}^{(1)}(x)}{dx}+\bar{\sigma}_{\mathrm{a}}\bar{\phi}^{(0)}(x)=\bar{Q}$$

The Drift-Diffusion Equation

- After combining resulting equations of order $1/\epsilon$, 1, and ϵ we arrive at the *drift-diffusion equation*

$$\frac{d}{dx}\left[-D(x)\frac{d\bar{\phi}^{(0)}(x)}{dx} + b(x)\bar{\phi}^{(0)}(x)\right] + \bar{\sigma}_{\mathrm{a}}(x)\bar{\phi}^{(0)}(x) = \bar{Q}$$

Diffusion — Drift

Discretizing the Drift-Diffusion Eq.

$$\frac{d}{dx}\left[-D(x)\frac{d\bar{\phi}^{(0)}(x)}{dx}+b(x)\bar{\phi}^{(0)}(x)\right]+\bar{\sigma}_{\mathrm{a}}(x)\bar{\phi}^{(0)}(x)=\bar{Q}$$

- We used a summation instead of an integral for calculating the macroscopic absorption cross section

$$\bar{\sigma}_a=\sum_{g=1}^{G}\sigma_a^g M^g$$

- M^g is the integral of the local Maxwellian between the energy bounds for group g

$$M^g=\int_{E_g}^{E_g-1}\mathrm{d}E\,M(E,T)$$

Discretizing the Drift-Diffusion Eq.

$$\frac{d}{dx}\left[-D(x)\frac{d\bar{\phi}^{(0)}(x)}{dx}+b(x)\bar{\phi}^{(0)}(x)\right]+\bar{\sigma}_{\mathrm{a}}(x)\bar{\phi}^{(0)}(x)=\bar{Q}$$

$$D(x)=\frac{1}{3\bar{\sigma}_{\mathrm{s}}}\left[\int_0^{\infty}\mathrm{d}E\,[1-\mathcal{S}_1]^{-1}M(E,T)\right]\equiv\frac{1}{3\bar{\sigma}_{\mathrm{s}}}\sum_{g=1}^{G}[I-\hat{\mathcal{S}}_1]^{-1}\vec{M}$$

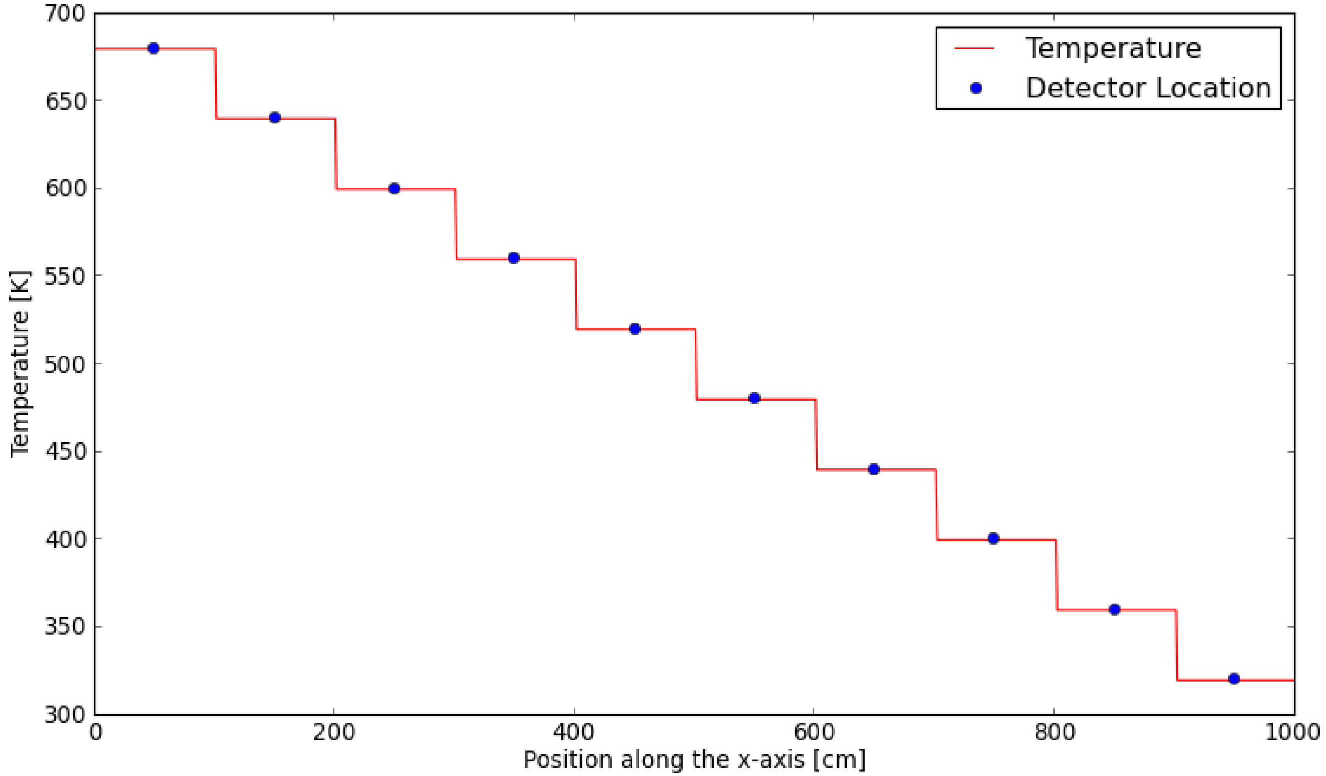
$$b(x)=-\frac{1}{3\bar{\sigma}_{\mathrm{s}}}\frac{dT}{dx}\left[\int_0^{\infty}\mathrm{d}E\,[1-\mathcal{S}_1]^{-1}\frac{\partial M}{\partial T}\right]\equiv-\frac{1}{3\bar{\sigma}_{\mathrm{s}}}\frac{dT}{dx}\sum_{g=1}^{G}[I-\hat{\mathcal{S}}_1]^{-1}\frac{\partial\vec{M}}{\partial T}$$

$$[I-\hat{S}_1]=\begin{bmatrix}1-\frac{1}{\sigma_s^1}\sigma_{s1}^{1\to1} & -\frac{1}{\sigma_s^1}\sigma_{s1}^{2\to1} & \cdots & -\frac{1}{\sigma_s^1}\sigma_{s1}^{G\to1}\\ -\frac{1}{\sigma_s^2}\sigma_{s1}^{1\to2} & \ddots & \cdots & -\frac{1}{\sigma_s^2}\sigma_{s1}^{G\to2}\\ \vdots & \cdots & \ddots & \vdots\\ -\frac{1}{\sigma_s^G}\sigma_{s1}^{1\to G} & \cdots & -\frac{1}{\sigma_s^G}\sigma_{s1}^{G-1\to G} & 1-\frac{1}{\sigma_s^G}\sigma_{s1}^{G\to G}\end{bmatrix}$$

First Benchmark for Drift-Diffusion Equation

- Verify whether this drift-diffusion equation is indeed an asymptotic limit to the neutron transport equation
- MCNP6 was used to construct the test problem
  - Graphite slab with a 1-eV neutron source uniformly distributed within the slab
  - Fixed linear temperature gradient across the slab
  - No incoming neutrons in MCNP6 simulation
    - Thus, zero-flux boundary conditions were used at both boundaries of the slab for the analytical model

Simplistic Linear Temperature Gradient



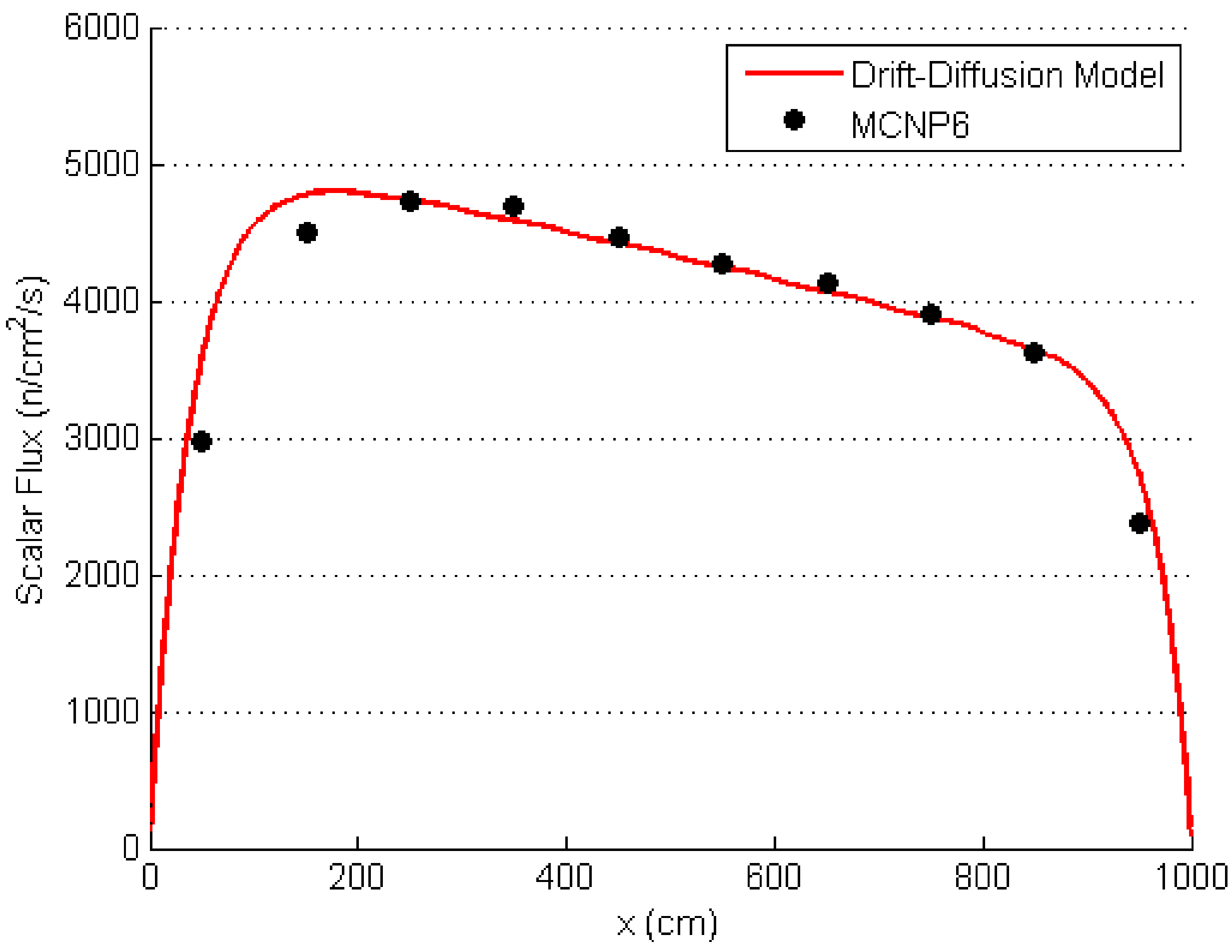
- NJOY-99 was used to generate continuous-energy cross sections at discrete temperatures for MCNP6 and corresponding multi-group cross sections for the analytical model
- Blue dots indicate “detector locations”
  - These are used to compare MCNP6 results to our analytical model

Group Structure

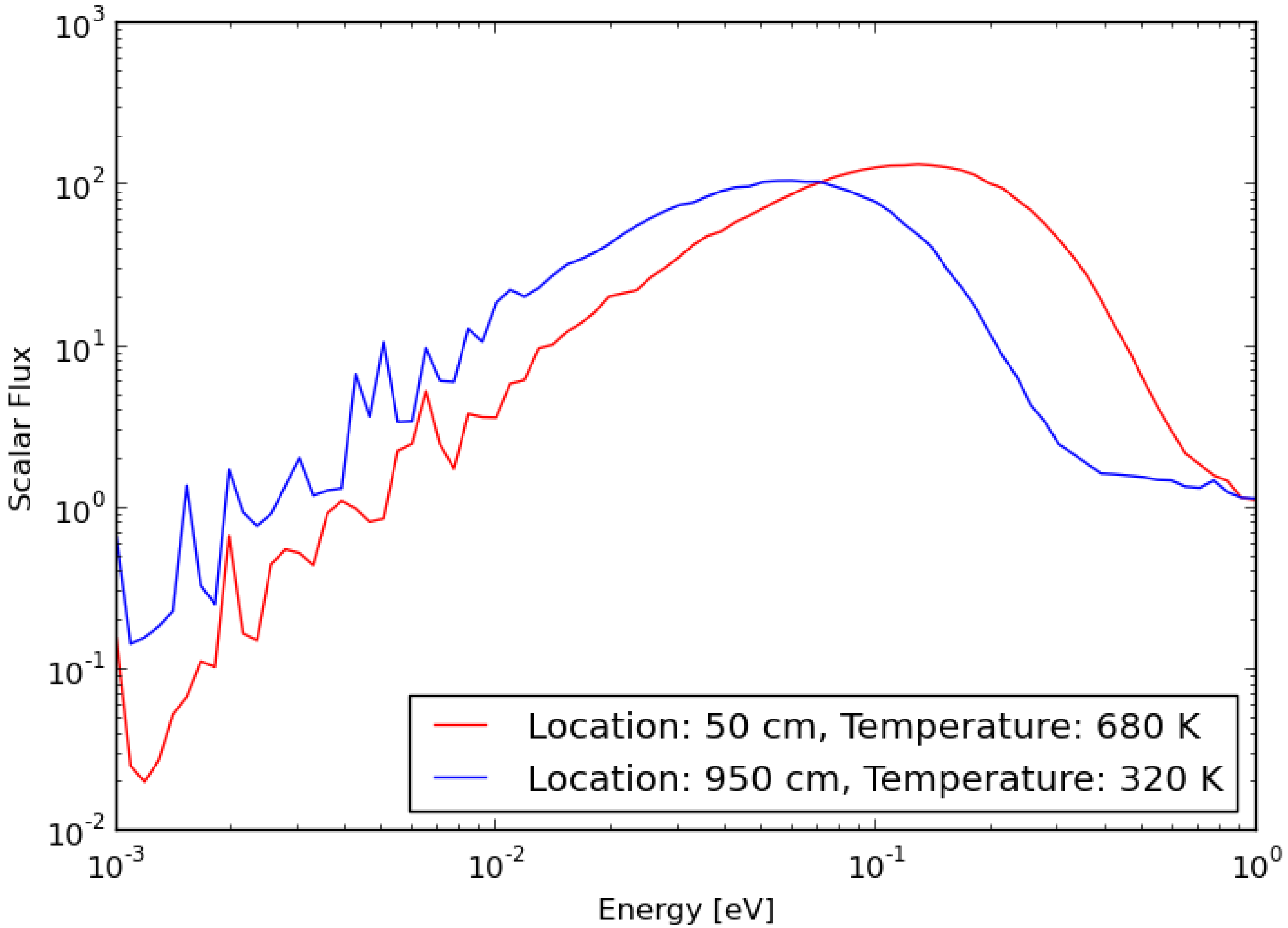
- The following group structure was used in the analytical models

Group	Lower Energy Bound (eV)	Upper Energy Bound (eV)
1	1.001	5.000
2	0.999	1.001
3	0.300	0.999
4	0.100	0.300
5	0.030	0.100
6	0.010	0.030
7	0.003	0.010
8	0.001	0.003
9	$1x10^{-4}$	0.001
10	$1x10^{-5}$	$1x10^{-4}$

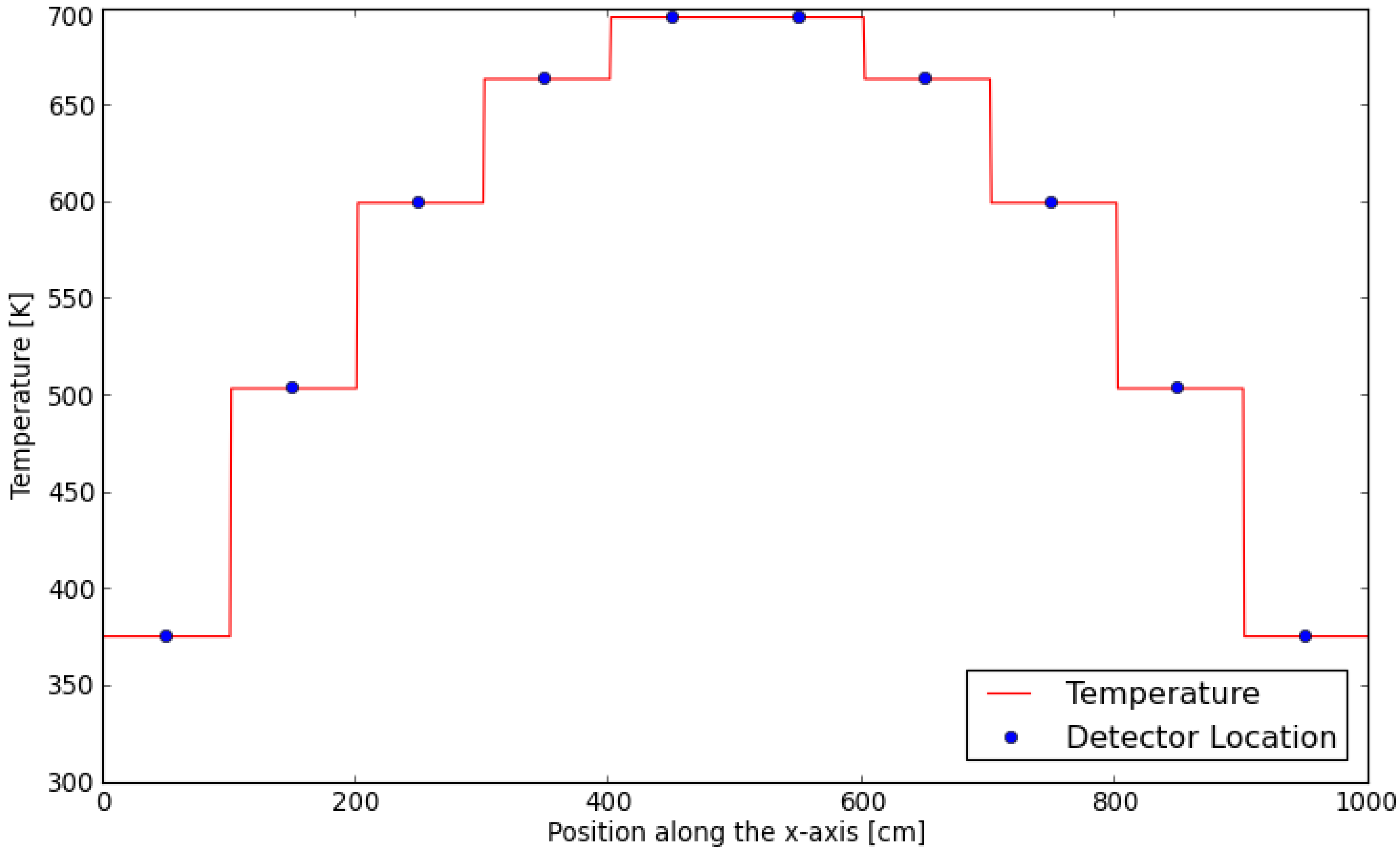
Results for Slab with Linear Temperature Gradient



Distribution of Neutron Energies in Different Slab Locations



Quadratic Temperature Gradient



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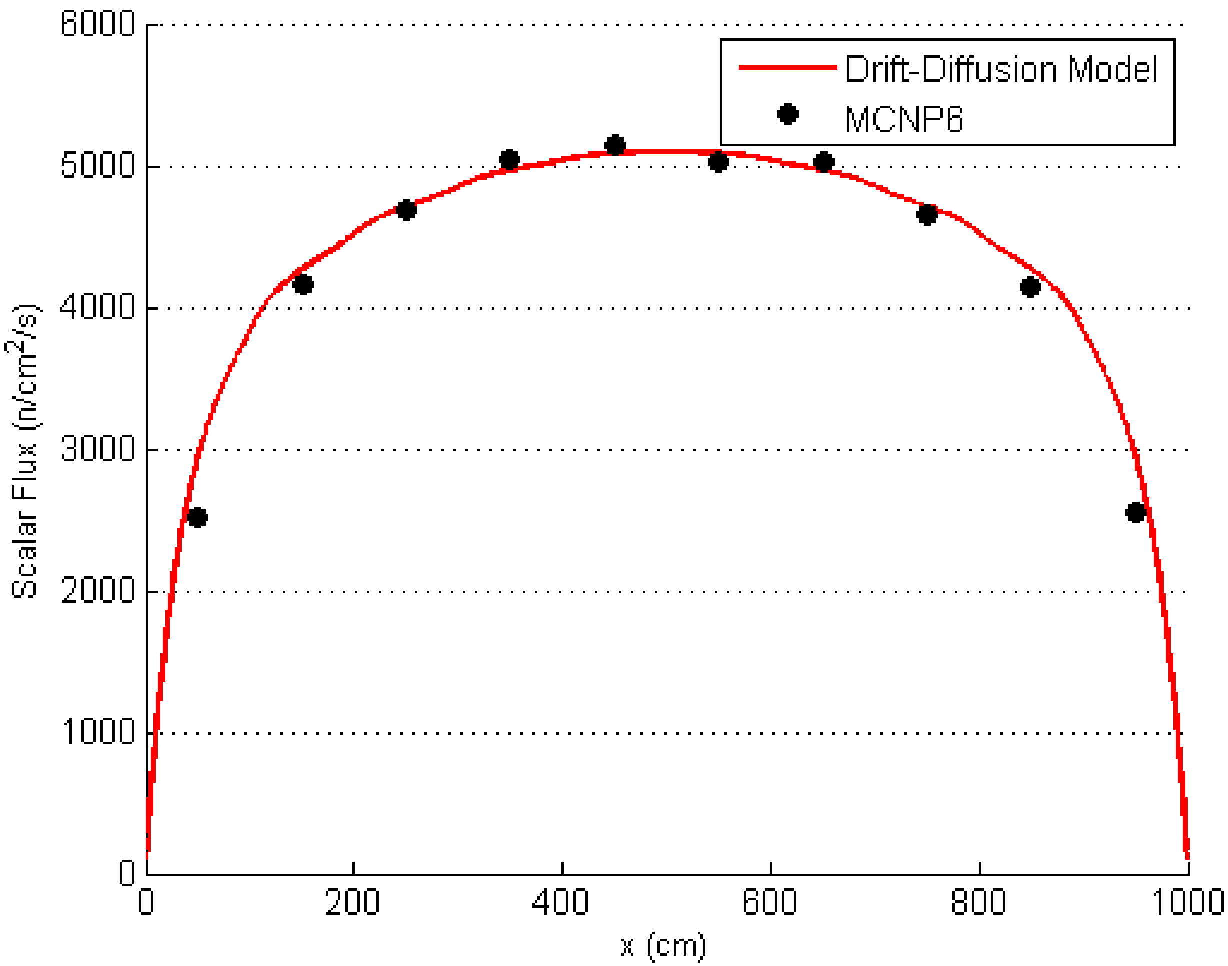

Conclusion

- Numerical results show that the transport of thermal neutrons in the absence of strong sources and absorbers can be described by a drift-diffusion model
- The model has a scalar flux that is a Maxwellian corresponding to the local material temperature

Future Work

- The drift-diffusion solution agreed with an MCNP6 solution in the interior of both slab-geometry problems
  - Near the boundary though, there was a discrepancy between the solutions
  - The derivation of appropriate boundary conditions, as well as initial conditions for the time dependent case, should be the topic of future work
- In the test problems involving a graphite slab, the value of the drift velocity was small compared to the diffusion coefficient
  - After deriving appropriate initial conditions and boundary conditions, we can experiment with problems with large drift velocities

QUESTIONS?