

Analytical Benchmark Solution for 1-D Neutron Transport Coupled with Thermal Conduction and Material Expansion

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ABSTRACT

In this work we present fully analytical solutions for a class of finite, homogeneous, 1-D slab benchmark problems with nonlinear temperature feedback effects. The proposed class of benchmarks include multiplicative 1-D neutron transport (limited to quasistatic S_2 with $\mu = \pm 1$) coupled with thermal conduction, convection, Doppler broadening, and expansion effects along the length of the slab. This class of benchmark models, along with the corresponding analytical solutions, are valuable for validating multiphysics analysis frameworks that support coupled neutronics/thermal/structural calculations. Analytical solutions for the benchmarks are obtained by introducing an ansatz that the equilibrium flux and temperature distributions in the slab have the same shape. Specific values for the total microscopic cross section, $\sigma_{t,0}$, and conductive heat transfer coefficient, h , that satisfy the assumed ansatz are then determined. A discussion of the procedure for generating benchmark models and analytical solutions is provided, along with numerical results for an example set of model parameters and thoughts on practical applications of the benchmarks for multiphysics code validation.

KEYWORDS: Multiphysics, analytical benchmark, eigenvalue

1. INTRODUCTION

Increased interest in the use of high-fidelity, coupled physics simulations for reactor analysis has created a need for accurate multiphysics benchmark solutions that can be used for code validation. These benchmark solutions do not necessarily have to reproduce a real reactor design or experimental measurement. However, meaningful benchmarks must capture the complexities of nonlinear feedback effects and subtle implications of various code-coupling strategies. Over the past several years, a series of analytical and semi-analytical multiphysics benchmarks have been developed for fixed-source neutron transport coupled with thermal/hydraulics [1], Doppler broadening [2-3], and depletion [4] feedback effects. In addition, benchmarks for “pseudo-eigenvalue” neutron transport with depletion [4] and Doppler broadening [5] feedback have also been reported. These pseudo-eigenvalue benchmarks provide an analytic solution for the neutron multiplication factor (k_{eff}) but not for the fundamental fission source distribution, which is arbitrary. Fewer analytical results are known for systems containing multiple concurrent feedback effects and/or neutron transport in a quasistatic multiplying system.

In 2021, Wang and Abdullatif investigated the stability of iterative numerical schemes applied to neutron transport with nonlinear temperature feedback [6]. Their work, which builds upon previous efforts from the 1970s and 1980s [7], considers temperature feedback effects in a multiplying, homogeneous slab due to heat conduction within the slab, convection from the ends of the slab, and thermal expansion of the slab material itself. By applying Fourier analysis, Wang and Abdullatif were able to derive results for the spectral radius of the iterative scheme as a function of the model parameters. Such results provide insight into the convergence properties of the numerical solution scheme but are restricted to trivial (*e.g.*, constant) solutions for the flux and temperature distributions within the slab.

In this work, we derive analytical solutions for the equilibrium material density, temperature, and neutron flux in a finite, multiplying, homogeneous, 1-D slab with nonlinear temperature feedback effects. The resulting analytical solutions are intended for use in the validation of multiphysics analysis frameworks that support coupled neutronics/thermal/structural calculations. The proposed validation model includes 1-D neutron transport (limited to S_2 with $\mu = \pm 1$) coupled with thermal conduction, convection, Doppler broadening, and expansion effects along the length of the slab. The solution methodology used in this work involves generating analytic solutions by making specific choices for certain physical parameters in the model – an approach which makes the resulting benchmark configurations especially easy to model in existing physics solvers without any changes to the underlying code. This solution approach should not be confused with the method of manufactured solutions (MMS), which seeks to generate analytic solutions through the specification of source terms and boundary conditions instead.

Note that the restriction to S_2 transport is often considered overly simplistic for radiation transport benchmarks. However, in this work, the objective is to find analytical solutions for three coupled solution fields (density, temperature, and flux) rather than just the radiation flux. To this end, the S_2 transport approximation allows simplification of the coupled system of multiphysics equations to a form that can be solved analytically. The resulting solutions are valuable for validating physics coupling implementations and can easily be adapted to Monte Carlo, S_N , or diffusion neutronics solvers – all of which are capable of handling S_2 transport without major modifications.

2. BENCHMARK DESCRIPTION

Consider a system consisting of one-speed neutrons traveling with directions $\mu = \pm 1$ in a 1-D slab with initial length L_0 , mass density ρ_0 , and zero-incident-flux boundary conditions on both sides. The slab is mechanically constrained and perfectly insulated in the transverse dimensions (y - and z -axes) but free to expand via frictionless sliding along the x -axis as the temperature of the slab changes. The ends of the slab are exposed to a convective heat sink at fixed (constant) temperature T_0 . The quasistatic equilibrium state of the slab is determined by three coupled equations that govern the flux, temperature, and material density profiles along the slab. Each of these differential equations are described in the following sections.

2.1. Thermal Expansion (Material Density)

The thermal strain at any location x in the slab is given by

$$\epsilon_x(T) = \int_{T_0}^T \alpha(T') dT' \quad (1)$$

where $\alpha(T)$ is the linear-expansion coefficient for the slab material. As the slab is heated, the differential length at every point in the slab will change in proportion to the local thermal strain

$$\ell(x) = \ell_0(\epsilon_x + 1), \quad (2)$$

where $\ell(x)$ and ℓ_0 are differential length elements in the heated and unheated slab, respectively, and thermal strain in the y and z dimensions has been neglected ($\epsilon_y = \epsilon_z = 0$). Growth of the slab must preserve total mass, which implies that the material density will change to compensate for slab expansion/contraction to satisfy mass conservation

$$\rho(x)\ell(x) = \rho_0\ell_0. \quad (3)$$

Substituting Eqs. (1) and (2) into (3) and rearranging gives an expression for material density as a function of the temperature distribution in the slab

$$\rho(x) = \frac{\rho_0}{\int_{T_0}^{T(x)} \alpha(T')dT' + 1}. \quad (4)$$

Assuming that the linear expansion coefficient is inversely related to the square root of the temperature

$$\alpha(T) \equiv \frac{1}{\sqrt{2 T_0 T}} \quad (5)$$

allows simplification of Eq. (4) to yield a solution for the material density profile along the slab length

$$\rho(x) = \rho_0 \sqrt{\frac{T_0}{T(x)}}. \quad (6)$$

The total length of the heated slab, L , can be defined implicitly in terms of the material density (Eq. (6)) by preserving total mass of the slab between the heated and unheated states, which can be expressed by the mass balance equation

$$\rho_0 \int_{-L/2}^{L/2} \sqrt{\frac{T_0}{T(x)}} dx = \rho_0 L_0. \quad (7)$$

2.2. Thermal Conduction and Doppler Broadening (Material Temperature)

The steady-state temperature distribution in the slab due to neutron heating is governed by the thermal conductivity equation

$$\frac{d}{dx} \left[\kappa(T) \frac{dT(x)}{dx} \right] + q \Sigma_t(x) \phi(x) = 0, \quad (8)$$

where $\kappa(T)$ is the thermal conductivity, q is the energy release per neutron interaction, $\phi(x)$ is the neutron flux, and Σ_t is the macroscopic total cross section for neutron interactions. The macroscopic cross section, in turn, is defined as

$$\Sigma_t(x) = M \sigma_t(T) \rho(x), \quad (9)$$

where $\sigma_t(T)$ is the microscopic total cross section with inverse-root Doppler broadening [2]

$$\sigma_t(T) = \sigma_{t,0} \sqrt{\frac{T_0}{T(x)}}, \quad (10)$$

with reference cross section $\sigma_{t,0}$ at temperature T_0 , $\rho(x)$ is the mass density, and M is the conversion between mass density and number density, given by $M = N_A/A$, where N_A is Avogadro's constant and A is the atomic mass of the constituent atoms/molecules in the slab material. Substituting the previous solution for density (Eq. (6)) into Eq. (9) yields an expression for the macroscopic cross section in terms of material temperature

$$\Sigma_t(x) = \frac{M\sigma_{t,0}\rho_0 T_0}{T(x)} = \frac{\Sigma_{t,0} T_0}{T(x)}, \quad (11)$$

where $\Sigma_{t,0} \equiv M\sigma_{t,0}\rho_0$ denotes the unheated macroscopic total cross section of the slab material.

The slab is exposed to a convective heat sink at temperature T_0 with heat transfer coefficient h at the ends ($x = \pm L/2$), which gives the boundary conditions

$$\pm \kappa(\pm L/2) \frac{dT}{dx} \Big|_{\pm L/2} + h[T(\pm L/2) - T_0] = 0. \quad (12)$$

Assuming that the thermal conductivity is a linear function of temperature,

$$\kappa(T) = \kappa_0 T(x), \quad (13)$$

and applying the definition for macroscopic cross section (Eq. (11)) allows the thermal conduction equation to be written in terms of the temperature and flux distributions

$$\frac{d}{dx} \left[T(x) \frac{dT(x)}{dx} \right] + \frac{q \Sigma_{t,0} T_0}{\kappa_0} \frac{\phi(x)}{T(x)} = 0, \quad \text{and} \quad (14)$$

$$\pm T(\pm L/2) \frac{dT}{dx} \Big|_{\pm L/2} + \frac{h}{\kappa_0} [T(\pm L/2) - T_0] = 0. \quad (15)$$

2.3. Radiation Transport (Neutron Flux)

The neutron flux distribution in the slab is governed by quasistatic transport on the line (*i.e.*, S_2 transport with $\mu = \pm 1$). The resulting transport equation and escape boundary conditions are

$$\frac{d}{dx} \left[\frac{1}{\Sigma_t(x)} \frac{d\phi(x)}{dx} \right] + (\lambda - 1) \Sigma_t(x) \phi(x) = 0, \quad \text{and} \quad (16)$$

$$\pm \frac{d\phi}{dx} \Big|_{\pm L/2} + \Sigma_t(\pm L/2) \phi(\pm L/2) = 0, \quad (17)$$

where λ is the combined inscattering and (quasistatic) fission source term, as defined by

$$\lambda \equiv \left(\frac{1}{k_{\text{eff}}} \frac{\nu \Sigma_f}{\Sigma_t} + \frac{\Sigma_s}{\Sigma_t} \right), \quad (18)$$

where ν is the average number of neutrons released per fission, k_{eff} is the multiplication factor necessary to achieve a steady-state neutron population in the slab, and Σ_f/Σ_t and Σ_s/Σ_t are the (constant) fractional probabilities of fission and isotropic scattering, respectively, per collision. The magnitude of the neutron flux is normalized to the total power output of the slab, P , through the integral relationship

$$P = \int_{-L/2}^{L/2} q \Sigma_t(x') \phi(x') dx'. \quad (19)$$

Substituting the previous definition for the macroscopic total cross section (Eq. (11)) into Eqs. (16) and (17) gives the S_2 neutron transport equations as a function of the temperature distribution in the slab

$$\frac{d}{dx} \left[\frac{T(x)}{\Sigma_{t,0} T_0} \frac{d\phi(x)}{dx} \right] + (\lambda - 1) \Sigma_{t,0} T_0 \frac{\phi(x)}{T(x)} = 0, \quad \text{and} \quad (20)$$

$$\pm \frac{d\phi}{dx} \Big|_{\pm L/2} + \Sigma_{t,0} T_0 \frac{\phi(\pm \frac{L}{2})}{T(\pm \frac{L}{2})} = 0. \quad (21)$$

3. ANALYTICAL SOLUTION

Equations (6), (14), and (20) govern the coupled mechanical, thermal, and nuclear processes for a 1-D slab subjected to the specified initial and boundary conditions (Eqs. (15) and (21)). In this Section, we seek analytical solutions for the material density, temperature, and neutron flux profiles in the slab that simultaneously (and consistently) satisfy the corresponding governing equations. The solution approach is to determine values for the physical constants σ_t and h that will allow the underlying differential equations (specifically Eqs. (14) and (20)) to reduce to forms that are easily solvable. Note that the existence of a solution obtained via this approach does not necessarily imply that the system can be solved for any combination of physical parameters.

We begin by noting that the differential equations for thermal conduction (Eq. (14)) and neutron transport (Eq. (20)) have similar forms, which suggests that it may be possible to select physical constants to manufacture a scenario where the flux and temperature distributions have the same shape. To this end, we introduce the ansatz that the flux and temperature distributions differ by a constant factor f , such that

$$T(x) = f \phi(x). \quad (22)$$

Substituting this ansatz into the definition for the macroscopic cross section (Eq. (11)) and applying the power normalization condition given in Eq. (19) yields a unique solution for the factor f ,

$$f = \frac{q \Sigma_{t,0} T_0 L}{P}. \quad (23)$$

Substituting Eqs. (22) and (23) into Eq. (11) gives an expression for the macroscopic cross section in terms of the neutron flux,

$$\Sigma_t(x) = \frac{P}{q L \phi(x)}. \quad (24)$$

3.1. Analytic Eigenvalue Solution for Neutron Flux

Substituting the assumed form of the cross section (Eq. (24)) into the transport equation and boundary conditions (Eqs. (16) and (17)) gives

$$\frac{d}{dx} \left[\phi(x) \frac{d\phi(x)}{dx} \right] = (1 - \lambda) \frac{P^2}{L^2 q^2} \quad (25)$$

$$\pm \frac{d\phi}{dx} \Big|_{\pm L/2} + \frac{P}{Lq} = 0. \quad (26)$$

The resulting differential equation can be solved by taking the integral of both sides of Eq. (25) with respect to x and applying separation of variables to yield the general form of the flux solution,

$$\phi(x) = \sqrt{x^2(1 - \lambda) \frac{P^2}{L^2 q^2} + 2C_0x + C_1}, \quad (27)$$

where C_0 and C_1 are arbitrary constants of integration. Note that the general form of the solution (Eq.(27)) includes 3 unknown constants (λ_1 , C_0 , and C_1) that must be determined based on the flux boundary conditions and amplitude. This can be done by noting that the model is symmetric about $x = 0$, which implies that the flux solution will satisfy the symmetry condition $\phi(x) = \phi(-x)$. Inspection of Eq. (27) reveals that flux symmetry is only satisfied when $C_0 = 0$. Therefore, the general flux solution for a slab requires $C_0 = 0$, which gives

$$\phi(x) = \sqrt{C_1 - \frac{(\lambda - 1)P^2x^2}{L^2q^2}}, \quad (28)$$

The remaining normalization coefficient, C_1 , can be expressed in terms of the maximum flux in the slab by evaluating Eq. (28) at $x = 0$ to yield

$$C_1 = \phi^2(0). \quad (29)$$

Thus, the coefficient C_1 acts as a flux scaling factor and does not affect the shape of the flux or reaction rate density (due to the inverse relationship between flux and total cross section). As a result, the value of C_1 is completely arbitrary. Substituting Eq. (29) into Eq. (28) and rearranging yields

$$\phi(x) = \phi(0) \sqrt{1 - \frac{(\lambda - 1)P^2x^2}{L^2q^2\phi^2(0)}}. \quad (30)$$

Note that Eq. (30) is identical to the formula for an ellipse, implying that the inverse flux cross-section feedback (Eq. (24)) yields an elliptical flux solution rather than the cosine solution normally seen in finite slab geometries with constant cross sections.

Finally, the eigenvalue λ can be determined by substituting Eq. (30) into either boundary condition ($x = \pm L/2$; see Eq. (26)) to give a second-order polynomial in λ ,

$$\lambda^2 - \lambda - \frac{4q^2\phi^2(0)}{P^2} = 0, \quad (31)$$

which can be solved via the quadratic formula,

$$\lambda = \frac{1}{2} \left(1 + \sqrt{1 + \frac{16q^2\phi^2(0)}{P^2}} \right). \quad (32)$$

Note that Eq. (32) omits the negative root, which is nonphysical.

3.2. Determination of Manufactured Parameters

With the analytical solutions for the neutron flux and eigenvalue established, we now seek to find values for the microscopic total cross section ($\sigma_{t,0}$) and convective heat transfer coefficient (h) such that the solution to the heat conduction equation (Eq. (14)) is a temperature distribution that also satisfies the flux/temperature ansatz established in Eq. (22). To determine the necessary parameters, we begin by applying Eqs. (22) and (23) to write the heat conduction equation (Eq. (14)) and associated thermal boundary conditions (Eq. (15)) in terms of neutron flux,

$$\frac{d}{dx} \left[\phi(x) \frac{d\phi(x)}{dx} \right] + \frac{P}{\kappa_0 L f^2} = 0, \quad \text{and} \quad (33)$$

$$\pm \frac{d\phi}{dx} \Big|_{\pm L/2} + \frac{h}{\kappa_0 f} \left(1 - \frac{T_0}{f\phi(\pm L/2)} \right) = 0. \quad (34)$$

For the ansatz to be satisfied, Eqs. (33) and (34) must be identical to the flux equation and boundary conditions given in Eqs. (25) and (26). Therefore, by matching coefficients between Eqs. (33) and (25) and expanding the previously established definitions of f and $\Sigma_{t,0}$, it follows that

$$\frac{P^3}{\kappa_0 L^3 q^2 (M\sigma_{t,0}\rho_0 T_0)^2} = (\lambda - 1) \frac{P^2}{L^2 q^2}, \quad (35)$$

which can be solved for $\sigma_{t,0}$ to give

$$\sigma_{t,0} = \frac{1}{M\rho_0 T_0} \sqrt{\frac{P}{\kappa_0 L(\lambda - 1)}}. \quad (36)$$

Similarly, matching coefficients for the boundary conditions (Eqs. (34) and (26)) and solving for h gives

$$h = \frac{\kappa_0 P f^2}{qL \left(f - \frac{T_0}{\phi(\pm L/2)} \right)}. \quad (37)$$

Note that the convective heat transfer coefficient is defined in terms of the flux solution at the ends of the slab. Substituting the previous solutions for f (Eq. (23)), $\phi(\pm L/2)$ (Eq. (30)), and $\sigma_{t,0}$ (Eq. (36)) into Eq. (34) gives the convective heat transfer coefficient in terms of more basic slab parameters

$$h = \left(\sqrt{\frac{L(\lambda - 1)}{\kappa_0 P}} - \frac{2T_0}{P} \right)^{-1}. \quad (38)$$

It is important to note that the convective heat transfer coefficient calculated with Eq. (34) is not guaranteed to be positive. In fact, negative values of h will occur when $T(\pm L/2) < T_0$. This is due to the assumption that the flux and temperature distributions have the same shape (Eq. (22)), which implies that there is net outflux of neutrons and heat from the slab at $x = \pm L/2$. However, if the temperature at the ends of the slab is less than the temperature of the heat sink then the slab will receive a net influx of heat through the ends, which implies that the derivative of the temperature distribution and flux distribution will have opposite signs. In the contrived solution this inconsistency is resolved by a negative heat transfer coefficient, which is nonphysical. Therefore, to ensure a physically meaningful solution, we impose the following constraint on the manufactured temperature distribution

$$T(\pm L/2) \geq T_0. \quad (39)$$

Substituting Eqs. (22) and (30) into Eq. (39) and rearranging gives a minimum condition for power (P) in terms of the other slab parameters

$$P \geq \frac{\lambda \kappa_0 T_0^2}{L(\lambda - 1)}. \quad (40)$$

Finally, we note that the flux and temperature solutions, along with all derived slab parameters, are defined in terms of the length of the heated slab, L , which, in turn, depends on the temperature/density distribution in the slab. The final length of the heated slab can be determined by substituting Eqs. (22) and (30) into Eq. (7), evaluating the resulting integral, and solving for L , which yields

$$L = \sqrt[3]{\left(\frac{L_0}{{}_2F_1\left(\frac{1}{4}, \frac{1}{2}; \frac{3}{2}; \frac{1}{\lambda}\right)} \right)^4 \left(\frac{\left(\frac{q^2 \phi^2(0)}{P(\lambda - 1)}\right) - \left(\frac{P}{4}\right)}{\kappa_0 T_0^2 \left(1 - \frac{1}{\lambda}\right)} \right)}, \quad (41)$$

where ${}_2F_1$ is the Gauss hypergeometric function.

3.3. Benchmark Generation/Solution Procedure

The results from the previous Sections prove the existence of analytical equilibrium solutions for a class of 1-D slab benchmark models with coupled mechanical, thermal, and nuclear feedback effects. Models in this class, along with their corresponding analytical solutions for material density, temperature, and flux profiles, can be generated and used for code validation by using the following procedure

- Select baseline values for the slab parameters $L_0, T_0, \rho_0, q, P, \kappa_0, v\Sigma_f/\Sigma_t, \Sigma_s/\Sigma_t, \phi(0)$, and A .
- Calculate the slab eigenvalue λ using Eq. (32).
- Calculate the equilibrium (*i.e.*, heated) slab length L using Eq. (41).
- Verify that selected power P satisfies the required minimum given in Eq. (40).
- Calculate the manufactured parameters $\sigma_{t,0}$ and h using Eqs. (36) and (38), respectively.
- Use assumed/manufactured values for $\alpha(T), \kappa(T), h, q, P, A$, and $\sigma_{t,0}$ as input for numerical solver(s) with specified boundary conditions and L_0, T_0 and ρ_0 (or $M\rho_0$ for number density) as initial conditions for the slab.

- Compare numerical solutions against analytical solutions for: $\phi(x)$ (Eq. (30)), λ (Eq. (32)), $\Sigma_t(x)$ (Eq. (24)), $T(x)$ (Eqs. (22) and (23)), $\rho(x)$ (Eq. (6)), and L (Eq. (41)).

4. NUMERICAL RESULTS

While the benchmark is analytic, it is convenient to have a set of ‘canonical’ parameters for consistent comparisons of accuracy between codes. A set of proposed canonical parameters are listed in Table I. Note that the table includes rows for $\nu\Sigma_f/\Sigma_t$ and Σ_s/Σ_t . These two quantities are not used in the generation of the analytic solution, but they are used to calculate the slab multiplication factor using Eq (18). The solution to the benchmark problem using these parameters is plotted in Figure 1. Included in the figure are the computed values of the derived parameters $\sigma_{t,0}$ and h for this problem, as well solutions for L and k_{eff} .

This analytic solution was confirmed via comparison against a naïve numerical implementation of the benchmark to confirm the results and the feasibility of its implementation. The numerical implementation used step differencing for transport, and a simple finite difference model for the thermal feedback. The implementation involved Picard iterations between transport and conductivity with additional nonlinear iterations for each conductivity solve. The numerical model converged to the correct eigenvalue and length to within a relative difference of 0.09% and 0.02% respectively when 1000 mesh points are used. As expected of the naïve implementation, these differences decrease linearly as the number of mesh points is increased, indicating that the numerical implementation indeed approaches the analytic solution.

5. CONCLUSIONS

In this work we present a fully analytical solution for a class of simplified 1-D slab benchmark problems with coupled feedback effects due to material growth, thermal conduction, and neutron transport/heating. The resulting benchmarks feature nonlinear relationships between each of the feedback effects and rely on a quasistatic (i.e., eigenvalue) formulation for the multiplicative neutron transport within the slab. The benchmark models are invaluable for validating multiphysics simulations that include coupled mechanical, thermal, and nuclear solvers. The analytical solution for the proposed class of benchmarks is obtained by introducing an ansatz that the equilibrium flux and temperature distributions in the slab will have the same shape. Specific values for the total microscopic cross section, $\sigma_{t,0}$, and convective heat transfer coefficient, h , that satisfy the ansatz are then determined by matching coefficients between the governing equations for heat conduction and radiation transport in the slab. A discussion of the procedure for generating benchmark models and analytical solutions is provided, along with thoughts on practical applications of the models for multiphysics code validation. Calculations for an example set of model parameters confirm that the numerical solutions approach the analytical solutions as the solution mesh is refined.

Table I. Numerical values for canonical parameters of the analytical benchmark problem.

Parameter	Value	Units
ρ_0	1.2	g/cm^3
L_0	100	cm
A	180	g/mol
T_0	293	K
q	1.0×10^8	eV
P	1.0×10^{22}	eV/s
κ_0	1.25×10^{19}	$\text{eV}/(\text{s cm K}^2)$
$\phi(0)$	2.5×10^{14}	$1/(\text{s cm}^2)$
$\nu\Sigma_f/\Sigma_t$	1.5	--
Σ_s/Σ_t	0.45	--

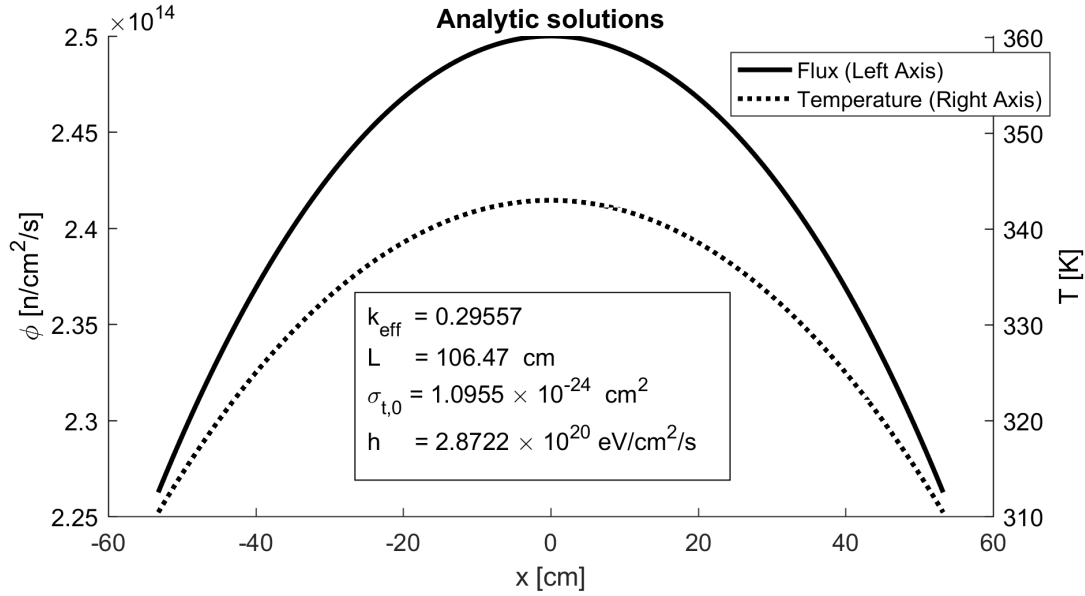


Figure 1. Analytic solution to the benchmark problem when using the parameters in Table I.

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